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Research

Review of SKB's Code Documentation and Testing

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SKI Perspective

Background

The Swedish Nuclear Waste Management Company (SKB) is currently developing the SR-Can safety assessment as a basis for their planned license application for an encapsulation plant. In the evaluation of long-term safety, numerous codes are used either as components in the overall risk assessment or as part of supporting safety arguments related to e.g. the containment of the engineered barrier system. An important consideration in the review of the SR-Can will be the quality of the documentation and testing of those codes.

Within this project, published information about SKB's documentation and testing of codes has been compiled. Each code is described and information regarding code usage as well as code verification and validation is discussed. Commonly used software quality standards are also described. In the SR-Can additional codes or updated versions of the codes discussed here might be used, so no complete evaluation could be done at this stage. However, the preliminary judgements made in this report, provides a starting point for the future review of SR-Can.

Relevance for SKI

The relevance of this report is mainly as a first preliminary evaluation of the status of SKB's code documentation and testing.

Results

The results show that there is a varying standard of code documentation and testing with some room for improvement in certain areas.

Future Work

In a future review of the SR-Can safety assessment, the codes covered by this work and their specific applications, calculation cases etc. need to be evaluated in detail. Related areas such as quality in the data handling for safety assessment calculations would also have to be scrutinised.

Project Information

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Project Identification Number: 200409101

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Executive Summary

SKB is in the process of developing the SR-Can safety assessment for a KBS 3 repository. The assessment will be based on quantitative analyses using a range of computational codes aimed at developing an understanding of how the repository system will evolve. Clear and comprehensive code documentation and testing will engender confidence in the results of the safety assessment calculations.

This report presents the results of a review undertaken on behalf of SKI aimed at providing an understanding of how codes used in the SR 97 safety assessment and those planned for use in the SR-Can safety assessment have been documented and tested.

Having identified the codes used by SKB, several codes were selected for review. Consideration was given to codes used directly in SKB's safety assessment calculations as well as to some of the less visible codes that are important in quantifying the different repository barrier safety functions. SKB's documentation and testing of the following codes were reviewed:

- COMP23 - a near-field radionuclide transport model developed by SKB for use in safety assessment calculations.

- FARF31 - a far-field radionuclide transport model developed by SKB for use in safety assessment calculations.

- PROPER - SKB's harness for executing probabilistic radionuclide transport calculations using COMP23 and FARF31.

- The integrated analytical radionuclide transport model that SKB has developed to run in parallel with COMP23 and FARF31.

- CONNECTFLOW - a discrete fracture network model/continuum model developed by Serco Assurance (based on the coupling of NAMMU and NAPSAC), which SKB is using to combine hydrogeological modelling on the site and regional scales in place of the HYDRASTAR code.

- DarcyTools - a discrete fracture network model coupled to a continuum model, recently developed by SKB for hydrogeological modelling, also in place of HYDRASTAR.

- ABAQUS - a finite element material model developed by ABAQUS, Inc, which is used by SKB to model repository buffer evolution.

- Poly3D - a displacement discontinuity model developed at Stanford University and used by SKB to study the effects of movement on fractures that intersect canister deposition holes.

- UDEC, 3DEC, FLAC, and FLAC3D - geotechnical models developed by HCItasca, and used by SKB in thermo-hydro-mechanical analysis of repository host rock.

- M3 - a multivariate mixing and mass balance model developed by SKB to study the evolution of groundwater composition.

The commercially available codes (CONNECTFLOW, ABAQUS, Poly3D, UDEC, 3DEC, FLAC, and FLAC3D) appear to have been subject to extensive testing, and the wide international usage of these codes offers a high level of confidence that they are fit for intended purpose. However, SKB has modified or developed some commercial codes in-house, and it is unclear whether these developments have become an integral part of, and have been subject to similar levels of testing as, the main code. Greater confidence in the applicability of the modified forms of these codes could be achieved if clear information on code usage and verification were available.

Varying standards of code documentation have been identified for the SKB codes COMP23, FARF31, PROPER, the analytical radionuclide transport code, DarcyTools, and M3. The recent DarcyTools reports are of a high standard, providing comprehensive information on the model basis, code usage, and code verification and validation. User's guides and verification reports should be developed for all of SKB's codes that are of a similar standard to the DarcyTools documents and are consistent with appropriate software quality assurance (QA) procedures.

To develop a greater understanding of suitable software documentation and testing standards, a brief review has been undertaken of software QA requirements in other radioactive waste disposal programmes. The review has provided useful insights into the type of code documentation that might be expected to accompany the submission of a repository safety assessment. The projects studied require that software is managed under a rigorous graded approach based on a software life-cycle methodology, with documentation requirements that include user's manuals and verification and validation documents. These requirements also include procedures for the use of external codes. Under the graded approach, reduced versions of the software life-cycle are adopted for simple codes, such as those that can be independently verified by inspection or hand calculation. SKB should provide details of its software QA procedures covering different categories of software (e.g., internal, commercial, academic, and simple codes).

In order to gain greater understanding and confidence in, and become more familiar with SKB's codes, SKI could consider testing some of SKB's codes against its own codes. This would also serve as a useful background to any future sensitivity analyses that SKI might conduct with these codes. Further, SKI could review its own software QA procedures and the required extent of documentation and testing of its own codes.

Contents

Review of SKB's Code Documentation and Testing

1 Introduction

1.1 Background

SKB is in the process of developing the SR-Can safety assessment for a KBS 3 repository, which will be used in SKB's application to build an encapsulation plant for spent nuclear fuel. The assessment will be based on quantitative analyses aimed at developing an understanding of how the repository system will evolve.

It is important that the codes used in a safety assessment are demonstrably fit for purpose. In particular, clear and comprehensive code documentation and testing can engender confidence in the results of safety assessment calculations. SKB is developing the system of computer codes used in the earlier SR 97 safety assessment for use in the SR-Can assessment. This report provides the results of a study undertaken by Galson Sciences Ltd on behalf of SKI aimed at providing an indication of how codes used in the SR 97 safety assessment and those planned for use in the SR-Can safety assessment have been documented and tested.

1.2 Approach

The project has involved four stages of work:

1. Identification of the computer codes that SKB used in SR 97. This activity aimed to cover codes that were used either directly or indirectly in the safety assessment.

2. Identification of the codes that SKB plans to use in SR-Can that are additional to or alternative to the codes used in SR 97.

3. Checking the level of documentation and testing of a selection of the codes planned for use in the SR-Can safety assessment.

4. Discussion of issues relating to the level of code documentation and testing that might be expected to accompany the submission of a repository safety assessment.

The work has been undertaken in consultation with SKB and in liaison with SKI, and has included a meeting with SKB and SKI staff (Stockholm, October 2004) to discuss interim findings.

1.3 Report Structure

Section 2 of this report discusses the findings from the first two stages of the project and lists the codes selected for more detailed consideration. The complete list of codes used by SKB in the SR 97 assessment and planned for use in the SR-Can assessment is provided in Appendix A. Section 3 provides a discussion of the testing and documentation of the selected codes. A discussion of software quality assurance standards and documentation requirements in nuclear waste management is presented in Section 4. A summary and conclusions are provided in Section 5.

2 Computer Codes Used by SKB

2.1 Identification of Codes

The main SR 97 post-closure safety reports (SKB, 1999a) and the SR 97 background report on processes in repository evolution (SKB, 1999b) provided the sources of material on code usage in the SR 97 safety assessment. These reports were studied with the aim of identifying the codes that had been used directly in the safety assessment as well as codes that had been used in analyses to support decision-making in the assessment.

The findings have been tabulated (see Appendix A) according to the scenario-based structure used to present the SR 97 assessment:
- initial state;
- base scenario;
- canister defect scenario;
- climate scenario;
- tectonics - earthquake scenario; and
- scenarios based on human actions.

Codes, their capabilities, and references to code usage have been listed for each scenario (where applicable) relating to the following processes:
- radiation-related;
- thermal evolution;
- hydraulic evolution;
- mechanical evolution;
- chemical evolution; and
- radionuclide transport.

The codes used directly in the SR 97 safety assessment (i.e. COMP23, FARF31, BIO42 and the PROPER control program) and the key codes that provided direct input to the assessment codes (e.g., HYDRASTAR and NAMMU) were clearly identified in the SR 97 post-closure safety reports. However, in most cases, the discussions of quantitative supporting studies in the SR 97 safety reports do not include mention of the codes used in the studies. In these cases, it was necessary to consult the cited reports to identify the code.

Information on the codes that SKB plans to use in the SR-Can safety assessment that are additional to or alternative to the codes used in SR 97 was extracted from the SR-Can planning report (SKB, 2003) and the SR-Can interim report (SKB, 2004) and added to Table A.1. The alternative codes to be used directly in future safety assessments have been identified in the SR-Can reports. However, as in the SR 97 reports, many of the codes to be used in supporting studies have not been identified.

Some major differences between the SR 97 and Sr-Can safety assessments in terms of code usage are as follows:

- The groundwater flow code HYDRASTAR is to be replaced by the two codes CONNECTFLOW (which is a coupling of the NAMMU continuum code and the NAPSAC discrete fracture network code) and DarcyTools.

- An integrated analytical radionuclide transport code will be run in parallel with COMP23 and FARF31.

- An integrated near-field evolution model will be used in support of the safety assessment codes.

- New ice sheet modelling is planned (covering permafrost, faulting, and hydrology).

- Modelling of fault and fracture displacements due to earthquakes using ABAQUS.

- Colloid transport modelling.

- A new approach to biosphere modelling will be undertaken using the codes Tensit and CoupModel.

Having established a list of codes used, or planned for use, by SKB, several codes were selected for review of their documentation and testing, as discussed in the following section.

2.2 Selection of Codes for Review

The role and origin of the codes used by SKB were considered in the selection of codes for further study in this project. The aim was to ensure consideration not only of codes used directly in SKB's safety assessment calculations but also of some of the less visible codes that are important in quantifying the different repository barrier safety functions. Also, codes developed by SKB and developed externally by commercial and academic organisations were chosen.

Such consideration led to the selection of the following codes for detailed review of the extent of their documentation and testing:

- COMP23 - a radionuclide transport model for the repository near-field (also known as NUCTRAN).

- FARF31 - a radionuclide transport model for the repository far-field.

- PROPER - a harness for executing probabilistic radionuclide transport calculations using COMP23 and FARF31.

- The integrated analytical radionuclide transport model that has been developed to run in parallel with COMP23 and FARF31.

- CONNECTFLOW - a discrete fracture network model nested in a continuum model (based on the coupling of NAMMU and NAPSAC), which is being used to combine hydrogeological modelling on the site and regional scales.

- DarcyTools - a discrete fracture network model coupled to a continuum model to be used in hydrogeological modelling alongside CONNECTFLOW.

- ABAQUS - a finite element material model with unsaturated fluid flow, which is used to model repository buffer evolution.

- Poly3D - a displacement discontinuity model used to study movement on fractures that intersect canister deposition holes.

- UDEC, 3DEC, FLAC, and FLAC3D - geotechnical models used in thermo-hydro-mechanical analysis of repository host rock.

- M3 - a multivariate mixing and mass balance model used to study the evolution of groundwater composition.

Section 3 presents the findings of the review of the above-mentioned codes.

3 Review of Code Testing and Documentation

The review sought to establish the extent to which the mathematical models and numerical solution techniques have been documented for the codes listed in Section 2.2. Also, the review aimed to summarise the types of code verification and validation studies, including code comparison exercises, checks against known analytical solutions for simplified geometries, and comparisons with measurements that have been reported for each code.

Documentation on each code was identified primarily by searching SKB's database of publications available via the SKB website. Reports not already available in Galson Sciences' library were obtained in electronic form directly from SKB's website, or were provided by SKB on request. SKB was also consulted directly for information on codes developed by commercial and academic organisations. Preliminary project findings were discussed at a meeting with SKB and SKI staff at SKB's offices in Stockholm on 27th October 2004, and further information on code documentation was provided by SKB.

The following sub-sections describe the findings with regard to the documentation and testing of the selected codes.

3.1 COMP23

COMP23 (known more generally as NUCTRAN) simulates radionuclide transport in the near field of a repository. COMP23 was the near-field code used in the SR 97 assessment (SKB, 1999a; Lindgren and Lindström, 1999), and it will be used by SKB in the SR-Can safety assessment (SKB, 2003; 2004).

3.1.1 Code Description

The COMP23/NUCTRAN code was described in a model validation document (Romero *et al*., 1995a). This model description was reproduced with minor revisions in the code user's guide (Romero *et al*., 1999).

In COMP23, radionuclides are assumed to leak from a damaged waste canister and diffuse through the repository barrier system into the surrounding fractured rock. The following processes are represented in coupled equations for the transport of concentrations of dissolved radionuclides and the mass of radionuclides in the solid phase:

- diffusion;
- dissolution;
- sorption (linear, reversible); and
- radioactive decay (chain decay).

Although a modified transport equation including advection at a constant fluid velocity is presented by Romero *et al*. (1999), the solution of the modified equation is not discussed.

The radionuclide transport equations are solved at a coarse scale using a compartment modelling approach. Analytical or semi-analytical solutions are used to obtain more detailed solutions in zones where finer solution grids would otherwise be needed. Such solutions are available for:

- Transfer of radionuclides by diffusion into water flowing in a fracture next to a modelled compartment. The derivation of the solution is not presented in the user manual. Instead, papers by Neretnieks (1979; 1982) are cited for a derivation of the solution from boundary layer theory. Application of this equivalent flow rate concept is discussed by Moreno and Gylling (1998).

- Transfer of solute by diffusion through a small area into a compartment of large volume. Insufficient information is provided to permit a full understanding of this "equivalent plug" model and no references to its derivation are provided.

- Transfer of solute by diffusion into a narrow fracture. An analytical solution is quoted for a transport resistance approximated by a plug of material at the mouth of the fracture. Neretnieks (1986) is cited for the derivation of this solution.

Diagrams would serve to communicate these analytical models more readily.

Different dissolution models may be used for the source term and instant release fractions may be specified. Details of the different dissolution models are provided, except where Werme *et al*. (1990) are cited for details of models of dissolution by alpha-radiolysis. The damage to the canister is modelled as a hole, which may be specified to grow.

An implicit solution method is used to solve the system of ordinary differential equations. The solution method is described only briefly by Romero *et al*. (1995a) and Romero *et al*. (1999). Kahaner *et al*. (1988) and SKB (1993) are cited for details of the technique.

Romero *et al*. (1999) provided a description of the NUCTRAN code, including information on each subroutine. There is a standalone version of NUCTRAN and a version called COMP23 that is implemented as a module of the PROPER package. PROPER is SKB's code package for performing radionuclide transport calculations in safety assessments (see Section 3.3).

3.1.2 Code Usage

Romero *et al*. (1999) provided information on running NUCTRAN as a submodel of PROPER. Romero *et al*. (1999) also provided an example of the use of NUCTRAN to calculate the transport of U-238 and Pu-239 in the near field of the KBS-3 repository. Input files were included.

Recently, a new version of the COMP23 user manual has been produced (Cliffe, 2004), but this manual has not been obtained for review under the present project.

3.1.3 Code Verification and Validation

There does not appear to be a single verification report that tests each feature or subroutine of the NUCTRAN code.

Romero *et al*. (1995a) stated that analytical solutions have been used to provide simple test cases. The TRUMP code has been used in a code comparison study for more complex problems (Romero *et al*., 1995b). Romero *et al*. (1995c) presented a comparison of NUCTRAN with TRUMP applied to the SFL3-5 repositories, in which diffusive and advective transport processes were tested. Input files were not provided. Both TRUMP comparisons highlighted the need for subdivision of modelled zones to reduce error in simulating the transport of short-lived radionuclides. Romero *et al*. (1995b) concluded that 20 to 30 compartments would be sufficient in many cases.

Gould *et al*. (1996) presented verification studies involving comparison of NUCTRAN with the one-dimensional transport codes INHOMOG and RARECAN for a high-level waste repository example. The study separately tested the parts of NUCTRAN that simulate:

- diffusion,
- the source term,
- radionuclide transfer from a compartment with diffusive transport to one with advective transport, and
- radionuclide release through a hole in a canister.

The studies again highlighted the need for subdivision of modelled compartments to reduce errors. The incorporation of a ‘plug’ component between the canister and bentonite backfill was required to ensure reasonable matches, although the specification of plug properties was not discussed. Reasonable matches were found for a case in which the hole size in the canister increased with time, but the single hole model in NUCTRAN was found to be a poor approximation to a case in which the canister contained many holes.

Lindgren and Widén (1998) examined the discretization of the COMP23 near-field model by dividing the near-field blocks into increasing numbers of compartments compared to the configuration used in the SR 95 assessment calculations. Release rates were found to be overestimated for short-lived radionuclides if the discretization was too coarse. Lindgren and Widén (1998) provided recommendations for the appropriate level of discretization.

Verification studies for the analytical solutions, such as the expression that represents radionuclide transport into a narrow fracture, and the alpha-radiolysis dissolution model have not been identified under this project.

The code does not appear to have been used in validation exercises involving experimental results. However, SKB (1999a) noted that Romero (1995) used the model to describe the propagation of a redox front at a natural analogue site, but this report has not been obtained under the current project. SKB (2004) stated that a model validity document for COMP23 will be produced.

3.1.4 Summary

NUCTRAN/COMP23 has been developed as a near-field transport model for use by SKB in repository safety assessments. A user's guide is available for the code.

COMP23 is based on a compartment model approach. The coarseness of the model can lead to inaccuracies, although SKB has undertaken studies to justify the level of discretization. Analytical solutions are used where more detailed solutions are required. Details of these analytical solutions are generally not provided in SKB's reports, but are available in the published literature.

No single verification report has been identified but some components of the code have been tested in code comparison studies. SKB plans to produce a model validity document for COMP23.

3.2 FARF31

FARF31 simulates radionuclide transport through fractured rock. FARF31 was used by SKB to calculate radionuclide transport in the far field of a repository in the SR 97 safety assessment (SKB, 1999a; Lindgren and Lindström, 1999), and it will be used similarly in the SR-Can safety assessment (SKB, 2003; SKB, 2004).

3.2.1 Code Description

A detailed description of the FARF31 code has been provided by Norman and Kjellbert (1990). More recently, Elert *et al*. (2004) provided a summary description of the code in a model validity document. The FARF31 model includes the following processes:

- advection of dissolved radionuclides through fractures in rock;
- dispersion of radionuclides in fractures;
- diffusion of radionuclides from fractures into the rock matrix with sorption on solid surfaces; and
- radioactive decay (including chain decay).

Norman and Kjellbert (1990) and Elert *et al*. (2004) provided descriptions of the FARF31 governing equations, initial conditions, and boundary conditions. FARF31 is based on a dual-porosity continuum approach in which a three-dimensional flow and transport system is constructed from a series of one-dimensional stream tubes. The one-dimensional advection-dispersion equation is solved with diffusion into the matrix perpendicular to the flow direction. Advection and diffusion are averaged across each stream tube. A version of FARF31 that includes radionuclide-specific values for matrix diffusivity was described by Eriksson *et al*. (1999).

The groundwater travel times are determined separately using a hydrological code. The model includes the concept of flow wetted surface area per unit volume of flowing water to capture the effects of flow along several flow paths in a single stream tube (Andersson *et al*., 1998).

Norman and Kjellbert (1990) provided comprehensive details of the numerical solution technique, which involves taking the Laplace transform of the equations and using a numerical algorithm to invert the transformed equations. A choice of three inversion algorithms is available.

3.2.2 Code Usage

FARF31 is a submodel of the PROPER control program (see Section 3.3). Norman and Kjellbert (1990) provided information on FARF31 code inputs and outputs, as well as a test example. More recently, a code user guide has been produced as an SKB progress report (Lindgren *et al*., 2002), although this document has not been obtained under the current project.

Elert *et al*. (2004) stated that a source code control system, which describes handling and update of the code, and test cases are available to check code updates and for use as templates (Lindgren *et al*., 2002).

3.2.3 Code Verification and Validation

A model validity document for FARF31 has been produced by Elert *et al*. (2004). They noted that it is not practical to validate FARF31 by comparing model predictions with results of field experiments on the timescales with which repository performance assessments are concerned. Instead, they proposed that FARF31 can be validated to some extent by justifying how component processes and parameters have been incorporated in the model.

Model verification was achieved by comparing FARF31 calculations with the results of analytical solutions to the advection-dispersion equation and results from another numerical model (the TRUMP code). FAFR31 was found to show good agreement with the results of the analytical solutions, although oscillatory solutions were produced in cases where radionuclide travel times were long and assumed depths of solute penetration into the matrix were low, resulting in matrix saturation.

TRUMP, a finite difference code, was used to solve advection-dispersion problems with matrix diffusion and sorption for comparison with FARF31. Elert *et al*. (2004) referred to an SKB progress report (Elert *et al*., 1998) for details of this code comparison exercise. Reasonably good agreement was achieved between the two codes. Elert *et al*. (2004) noted that further code testing is discussed in another SKB progress report (Elert *et al*., 2001).

3.2.4 Summary

FARF31 has been developed as a far-field transport model for use by SKB in repository safety assessments. A model validation and verification document and a user's guide have been produced for FARF31. A detailed description of the governing equations and solution technique is also available. Several FARF31 reports, including the user's guide, are SKB progress reports that are not listed as publications on the SKB website.

FARF31 has been verified successfully, although oscillatory solutions may be generated in some cases. Validation has been based on justification of modelling assumptions rather than on comparison with field experiments because of the impracticality of undertaking the latter on timescales relevant to repository performance assessments.

3.3 PROPER

PROPER (PRObabilistic PERformance assessment) is a control program that executes the chain of sub-models in SKB's radiological consequence modelling system. PROPER was used in the SR 97 safety assessment (SKB, 1999a; Lindgren and Lindström, 1999). PROPER is not discussed in the SR-Can planning and interim reports (SKB, 2003; SKB, 2004).

3.3.1 Code Description

PROPER is a code that allows the user to link submodels describing radionuclide transport, such as COMP23 and FARF31. The PROPER Monitor controls the execution of the system of submodels. Each submodel is either an internal FORTRAN subprogram or an external FORTRAN program. The PROPER Monitor may be used to create a complete problem model. A user's manual (Kjellberg, 1999a), a submodel designer's manual (Kjellberg, 1999b) and a programmer's manual (Kjellberg, 1999c) are available for the PROPER code.

Kjellberg (1999a) provides a general description of PROPER. PROPER may be used to run deterministic or probabilistic calculations. For probabilistic calculations, input parameters may be defined as distributions rather than fixed values in order to capture parameter uncertainties. The input values are then sampled for each of many realisations using a Monte Carlo sampling procedure.

Kjellberg (1999c) provides information on the PROPER subprograms.

3.3.2 Code Usage

Kjellberg (1999a) provides general information on using PROPER, although specific guidance on using PROPER to run the radionuclide transport codes used in SKB's performance assessments calculations does not appear to be available.

3.3.3 Code Verification and Validation

No information on testing or validating the PROPER code has been identified.

3.3.4 Summary

The PROPER control program was used in the SR 97 safety assessment but it is not clear if it will be used in the SR-Can safety assessment. A user's manual is available, but information specific to using PROPER in safety assessments, and information on testing and validating PROPER, has not been identified.

3.4 Integrated Analytical Radionuclide Transport Model

SKB has recently developed simplified analytical near-field and far-field transport models (Hedin, 2002). The analytical models will be used to calculate radionuclide transport and dose consequences for many variant and residual cases in the SR-Can safety assessment (SKB, 2004).

3.4.1 Code Description

Hedin (2002) provided a detailed description of the near-field and far-field analytical models. The near-field model assumes diffusional transport of dissolved radionuclides through a buffer following release from a canister, with sorption occurring in the buffer. The geosphere model assumes radionuclide transport by advection in fractures and diffusion in the rock matrix, with sorption occurring in the fractures and the matrix.

Hedin (2002) presented details of the techniques used to solve the near-field and far-field mass transport equations. Direct solutions were developed using the method of Laplace transforms. Different solutions were derived for far-field mass transport depending on the form of radionuclide release from the buffer to the geosphere. A constant inlet solution is assumed for situations in which radionuclide release from the near field is slowly changing. Otherwise a pulse inlet solution is assumed.

Peak annual doses in the biosphere are calculated by multiplying peak releases from the geosphere by dose conversion factors.

Hedin (2003) noted that the code may be executed probabilistically using Microsoft Excel in conjunction with the Palisade Corporation's @Risk software. Hedin (2003) found that calculation speed using the analytical models is increased by about three orders of magnitude compared to SKB's corresponding numerical models.

3.4.2 Code Usage

SKB (2004) noted that the analytical models use the same input data as the corresponding numerical models. However, no guidance on using the code has been identified under this project.

3.4.3 Code Verification and Validation

Hedin (2002) verified the analytical approach by comparing results with those of SKB's numerical models for the near field and far field. Calculated peak releases from the buffer and from the geosphere using the analytical models were found to agree with results generated by the numerical models to within an order of magnitude.

SKB (2004) noted that the use of two complementary sets of models, building on the same concepts and using the same input data, provides quality assurance for the handling of probabilistic calculations.

3.4.4 Summary

SKB has developed efficient analytical near-field and far-field transport models that will be used in the SR-Can safety assessment in support of the main performance assessment codes. Details of the analytical models have been provided in a paper published in the Nuclear Technology journal. However, SKB does not appear to have produced a user guide and verification report for the model, although a verification exercise was presented in the Nuclear Technology paper.

3.5 CONNECTFLOW

CONNECTFLOW (CONtinuum and NEtwork Contaminant Transport and FLOW) has been developed for modelling groundwater flow and transport in porous and fractured media. SKB plans to use CONNECTFLOW for groundwater flow modelling in the SR-Can safety assessment in place of the HYDRASTAR stochastic continuum model that was used in the SR 97 assessment. CONNECTFLOW is also being used by SKB for site analysis in conjunction with the DarcyTools groundwater flow and transport code. Jaquet and Siegel (2003; 2004) and Hartley (2004) presented recent applications of CONNECTFLOW that are discussed in the SR-Can interim report (SKB, 2004).

CONNECTFLOW is produced by Serco Assurance and information on the code is available via the website www.connectflow.com.

3.5.1 Code Description

Marsic *et al*. (2001) reported that SKB had the following options for formally nesting a site-scale model within a regional scale model:

- Use the NAMMU continuum model to nest a refined site-scale model within a coarser far-field model.
- Use the CONNECTFLOW model with a Discrete Fracture Network (DFN) site-scale model nested within a continuum far-field model.

The first of these approaches has been demonstrated in several SKB studies (e.g., Marsic *et al*., 2001; Marsic *et al*., 2002). NAMMU has also been used regularly in previous safety assessment studies such as SR 97 for regional-scale analyses.

The second approach was developed to fulfil the need to embed a detailed site-scale fracture model within a regional-scale continuum model. CONNECTFLOW combines the two models NAPSAC and NAMMU to allow unified DFN and EPM (effective porous medium) modelling. The DFN code NAPSAC models groundwater flow and transport in fractured rock.

SKB (2003) reported that CONNECTFLOW includes the following capabilities:

- Nested continuum and discrete fracture models on all scales relevant to repository assessment with continuity preserved.
- Transient, density-dependent simulations. The code may be used to address issues such as the potential accumulation of high-salinity pockets beneath permafrost.
- A continuum representation of the engineered systems (tunnel and deposition holes) within a discrete representation of the fracture network on repository and block scales, thus providing more detailed input to the near-field model COMP23.

SKB (2003) also noted that some aspects of CONNECTFLOW required further development and testing, including:

- Simulation of wells, for example, to evaluate the capture zone for migrating radionuclides and dilution in the well.
- Treatment of surface hydrology.

The NAMMU governing equations for mass conservation, fluid flow (Darcy's law) and salt transport, and the solution technique (Newton-Raphson iteration or fully implicit Crank-Nicholson), are summarised briefly in Marsic *et al*. (2002). SKB has cited Hartley *et al*. (2001) for details of the development of the CONNECTFLOW model. Hartley and Holton (2003) provide summary information on the equations implemented in CONNECTFLOW to model fluid flow and mass transport, and the method for connecting the fracture network and porous medium models.

3.5.2 Code Usage

Hartley and Holton (2003) provided an overview of the CONNECTFLOW user interface, and information on the steps involved in setting up a CONNECFLOW model. They referred to a CONNECTFLOW installation and running guide and a CONNECTFLOW reference manual.

Hartley and Holton (2003) also referred to the iCONNECT club (integrated CONtinuum and NEtwork approach to groundwater flow and Contaminant Transport), which is intended to provide a forum for application and enhancement of CONNECTFLOW, especially for those involved in evaluating the geosphere as part of repository safety assessments.

3.5.3 Code Verification and Validation

The Serco Assurance website reports that NAMMU, NAPSAC and CONNECTFLOW have been developed over a period of more than 10 years, and have been verified extensively. Serco Assurance requires that rigorous tests are applied to each new code release. CONNECFLOW is developed under a quality system that meets the international ISO 9001 standard and the TickIT guidelines (see Section 4.1.1).

NAMMU has been used in the HYDROCOIN verification exercise and the INTRAVAL validation exercise, and NAPSAC has been used in the STRIPA project. CONNECTFLOW has been used in several projects for the deep disposal of radioactive and toxic waste, and contaminated land. Hartley and Holton (2003) referred to a CONNECTFLOW verification document.

SKB is applying the two groundwater flow codes CONNECTFLOW and DarcyTools in the SR-Can site characterisation studies using two independent modelling teams (SKB, 2003). SKB (2003) considered that the production of similar results by two independent codes/teams would lend credibility to the analysis and that independent modelling efforts would provide quality control on data handling and modelling practice.

3.5.4 Summary

CONNECTFLOW has been developed by Serco Assurance, and represents the connection of two component models, NAPSAC (DFN model) and NAMMU (EPM model), which have been available separately for over 10 years. CONNECTFLOW may be considered to be fit-for-purpose with a high level of confidence.

Recently, SKB's use of CONNECTFLOW to nest a refined site-scale model within a coarser far-field model has been reported by Jaquet and Siegel (2003; 2004) and Hartley (2004) and is discussed in SKB (2004).

Detailed information on the CONNECTFLOW model and its verification and validation may be obtained from Serco Assurance.

3.6 DarcyTools

DarcyTools was developed by SKB and CFE (Computer-aided Fluid Engineering) for simulating fluid flow and transport in porous and fractured media. DarcyTools is described in detail in three reports recently released by SKB: a description of the model concepts, equations, and solution methods (Svensson *et al*., 2004); a user's guide (Svensson and Ferry, 2004); and a verification and validation report (Svensson, 2004).

DarcyTools is being used by SKB for site analysis in conjunction with the groundwater flow and transport code CONNECTFLOW (SKB, 2003; 2004).

3.6.1 Code Description

DarcyTools represents SKB's progression from the Computational Fluid Dynamics (CFD) code Phoenics (SKB, 2003; Svensson *et al*., 2004), although the relationship between the two codes is unclear.

The theoretical basis for DarcyTools has been presented in Svensson *et al*. (2004). This report provides a clear description, including several helpful illustrations of how fracture systems are represented in the model. A useful example of the GEHYCO method for determining fluxes across cell walls that are intersected by conductive features (such as fractures and faults) is provided in an appendix. The report also contains a good description of the FRAME subgrid model for determining the effects of the storage volume in a grid element.

Elsewhere, the report presents the governing equations for mass conservation, mass transport, heat conservation, and Darcy flow, and describes two transport options: particle tracking using the PARTRACK algorithm and an advection/dispersion option. DarcyTools also includes a novel, well-described, approach to determining the groundwater table.

An appendix in Svensson *et al*. (2004) contains a comprehensive description of the integration of the differential equations and their solution using the MIGAL solver in the SOLVE code. MIGAL is a coupled algebraic multigrid solver for computational fluid dynamics applications. Reference is made to the MIGAL developer's website for further information (www.mfrdc.com).

3.6.2 Code Usage

The DarcyTools user's guide (Svensson and Ferry, 2004) describes how input data can be specified with data statements in the Compact Input File (CIF). The CIF is explained in detail and each command in the CIF is defined with an example of its use. However, Svensson and Ferry (2004) also noted that a few components of the DarcyTools source code are user-accessible:

- A Fortran input file (fif.f) may be used to specify parameters in a more detailed form than is available through the CIF, such as transient boundary conditions. Use of the fif.f gives the user more control but requires an understanding of the code and Fortran programming. The fif.f file may be used in situations where transient source terms, fluid properties as a function of variables, and boundary conditions as a function of time and space are required. The user's guide includes an empty fif.f, which comprises a number of subroutines that must be programmed. Several examples of the use of the fif.f are provided.

- A property generation Fortran file (prpgen.f) may be used for advanced fracture network representation. An example of the prpgen.f file is provided.

The user's guide includes a description of the code operational structure, information on hardware and operating systems, and details of the installation directory and file structure.

An informative demonstration case is provide, which includes the features and processes relevant to an underground research laboratory, with a resemblance to Äspö albeit in a simplified form. This example provides example usage of the fif.f and prpgen.f in a realistic situation.

3.6.3 Code Verification and Validation

The DarcyTools verification and validation report (Svensson, 2004) includes a discussion of the processes and actions involved in confidence building. It is acknowledged that DarcyTools is a new code with many advanced features, with only a few applications to date, implying that confidence building is at an early stage.

Svensson (2004) included many verification studies aimed at testing:
- numerical methods;
- porous medium flow algorithm;
- fracture fluid flow algorithm;
- transport algorithms; and
- salinity and temperature gradient algorithms.

Svensson (2004) found all the tests to be satisfactory. However, the numerical solution to the advection/diffusion equation does produce numerical diffusion.

Svensson *et al*. (2004) and Svensson (2004) argued that validation of the Phoenics code is relevant to the validation of DarcyTools because the codes are based on the same methods for representing fracture networks and other processes, and the codes have been shown to give similar results. Svensson (2004) contains several validation tests for Phoenics and DarcyTools, covering:

- the site scale;
- the laboratory scale;
- the repository scale; and
- the experimental scale.

The verification and validation tests appear to address the range of processes included in the DarcyTools model.

Svensson *et al*. (2004) includes a grid refinement study that gives a good illustration of code discretization errors.

As noted in Section 3.2.3, SKB (2003) considers that the use of the two groundwater flow codes CONNECTFLOW and DarcyTools in the SR-Can site characterisation studies will lend credibility to the analysis.

3.6.4 Summary

DarcyTools has been developed recently by SKB for groundwater flow and radionuclide transport analysis, and is being used in conjunction with the groundwater flow and transport code CONNECTFLOW. Recently published reports have provided comprehensive descriptions of the DarcyTools model concepts, equations, solution methods, code usage, and code verification and validation.

The DarcyTools reports acknowledge that the code is relatively new and that further application is required to build confidence in its usage.

A high level of expertise would be required to run DarcyTools if the more advanced features were to be implemented. Use of the Fortran input file (fif.f) and the property generation Fortran file (prpgen.f) requires a thorough understanding of the code and Fortran programming.

3.7 ABAQUS

ABAQUS is a finite element code that was originally designed for non-linear stress analysis, but has been extended to model a range of processes in different materials in a three-dimensional geometry. ABAQUS has been used by SKB over many years in studies of the thermo-hydro-mechanical (THM) evolution of the canister deposition hole buffer in the KBS 3 repository concept (e.g., Pusch and Börgesson, 1992; Börgesson, 1993; Börgesson and Hernelind, 1999; Börgesson *et al*., 2003).

ABAQUS is produced by ABAQUS, Inc. and information on the code is available via the ABAQUS website at www.abaqus.com.

3.7.1 Code Description

In reports on studies using ABAQUS, SKB generally has referred to ABAQUS manuals for detailed information on the model and its theoretical background (e.g., Hibbit *et al*., 1993). However, Börgesson and Hernelind (1999) presented the general equations of the ABAQUS hydro-mechanical and heat transfer models used in the buffer analysis.

The hydro-mechanical model consists of a porous medium and a wetting fluid and is based on:

- general stress equilibrium (a Drucker Prager plasticity model) and effective stress equations (poro-elastic) with a moisture swelling correction;
- an energy balance equation;
- constitutive equations for separate solid and liquid phases including thermal expansion;
- fluid mass conservation and flow equations (Darcy's law) in a partially saturated medium; and
- saturation-dependent diffusive vapour movement driven by a temperature gradient.

The temperature-driven water vapour flow code was developed separately by SKB and is not part of the ABAQUS code. Börgesson and Johannesson (1995) discussed the water vapour transport equation and noted that the code development was carried out by the company FEM-Tech AB on behalf of SKB. However, information on how the subroutine was coded and is integrated into ABAQUS applications has not been provided. Börgesson and Hernelind (1999) considered that the mechanical and vapour flux parts of the model needed to be improved.

The heat transfer model, which is not coupled directly to the hydro-mechanical model, involves:

- an energy balance equation; and
- constitutive equations for heat transfer (thermal conduction).

Börgesson and Hernelind (1999) coupled the hydro-mechanical and thermal models by running the models alternately and updating the material parameters (heat conductivity and specific heat as functions of saturation and water content) until convergence was achieved.

In another study, Börgesson *et al*. (1995) presented a model of the THM behaviour of MX-80-type buffer material. A mechanical model called CLAYTECH/S/A was implemented and coded in ABAQUS.

The finite element numerical solution technique used in ABAQUS has not been described in any of the reports studied in this project. Such information could, most likely, be obtained from the code developers, ABAQUS, Inc.

3.7.2 Code Usage

Details of code input and output handling and guidance on running ABAQUS have not been provided in the reports studied in this project. Such information is likely to be available from the code developers, ABAQUS, Inc, although it is unclear whether this would include information on running the subroutine for water vapour transport that was developed by SKB.

Lists of the ABAQUS parameter requirements for a buffer material model and examples of finite element solution meshes are provided in several SKB reports. Börgesson and Hernelind (1999) presented a solution mesh (of about 2,600 elements) for THM analysis of an axially symmetric deposition hole in which backfill material, a canister, the rock matrix and a damage zone around the deposition hole were modelled. Fractures intersecting the deposition hole were included in some studies. In a similar study, Börgesson and Hernelind (1997) used a solution mesh of 3,960 elements for an axially symmetric deposition hole. Börgesson *et al*. (2003) used a mesh of about 500 elements to represent the buffer and canister in a three-dimensional analysis of the effects of rock shearing. None of these reports discussed the rationale for selecting the number and distribution of mesh elements.

3.7.3 Code Verification and Validation

ABAQUS has had a broad user base for over 20 years, which implies that the code has been subjected to much testing.

Application of ABAQUS to THM modelling of the buffer evolution requires calibration tests to be carried out in order to evaluate parameters that cannot be measured directly in the laboratory (drying and wetting tests, swelling pressure tests, water uptake tests, and temperature gradient tests). The results of calibration tests have been provided by Börgesson and Johannesson (1995), although further testing was recommended. Börgesson and Hernelind (1999) described some of the calibration results as preliminary, because the material initial conditions varied between some tests, and concluded that new tests should be performed.

The water vapour flow component of the code was not validated by Börgesson and Johannesson (1995). However, temperature gradient (or moisture redistribution) tests were used by Börgesson and Hernelind (1999) and Börgesson and Hernelind (1997) to calibrate vapour flow diffusivity.

The ABAQUS code was also used in the CATSIUS CLAY project in code benchmark tests (Börgesson and Hernelind, 1997). Calculations of the water saturation phase of a reference clay were undertaken. Measured and calculated water inflows and water ratios were found to give reasonable agreement. However, calculated swelling pressures did not agree well with measured values. Börgesson and Hernelind (1995) similarly found disagreements between measured and calculated values of pressure in their analysis of the Big-Ben experiment to investigate the THM behaviour of buffer material in a deposition hole. The CLAYTECH/S/A buffer material model developed by Börgesson *et al*. (1995) and incorporated in ABAQUS was tested by simulating four laboratory tests (swelling/compression tests and triaxial tests). Again, problems in achieving reasonable estimates of swelling were reported.

3.7.4 Summary

ABAQUS is produced by ABAQUS, Inc., a provider of software for finite element analysis worldwide. The code has had a broad user base for over 20 years. Therefore, ABAQUS may be considered to be fit-for-purpose with a high level of confidence.

However, SKB has developed a number of code modules independently, such as a temperature-driven water vapour flow code and a mechanical model of a clay buffer, for use in conjunction with ABAQUS. It is unclear how these modules have been integrated with ABAQUS, whether any information in the use of these modules is available, or the extent to which these modules have been tested.

3.8 Poly3D

Poly3D is a three-dimensional displacement discontinuity code that has been used by SKB for studying the effects of fracture displacements on the integrity of canisters in disposal holes.

Poly3D was developed at Stanford University and information on the code can be found at the http://pangea.stanford.edu/research/geomech/.

3.8.1 Code Description

SKB generally cites Thomas (1993) for details of the Poly3D model, but this Stanford University thesis has not been obtained under the current project. The Stanford University website provides a brief overview of Poly3D. The code calculates the quasi-static displacement, strain and stress fields in a linear-elastic, homogeneous and isotropic medium using planar, polygonal elements of displacement discontinuity and the boundary element method (BEM). A polygonal element may represent some portion, or all, of a fracture or fault surface. The displacement discontinuity (fracture aperture or fault slip) is constant on each element, but multiple elements may be used to model an arbitrary number of mechanically-interacting fractures or faults with non-uniform opening and/or slip distributions. Irregular, curved faults and joints can be modelled.

La Pointe *et al*. (1997) noted that by ignoring visco-elastic behaviour, Poly3D is likely to overestimate displacements and stresses.

La Pointe *et al*. (1999) presented a modification to the Poly3D code. Poly3D originally calculated displacements at the mid-point of fractures. The modified code incorporates a solution for the variation in displacement along a fracture, with the maximum displacement occurring at the fracture mid-point. Pollard and Segall (1987) is cited for the expression giving displacements along a fracture.

3.8.2 Code Usage

No information on running Poly3D has been identified under this project, although the SKB reports on Poly3D applications provide an indication of the requirements of the code.

Poly3D requires specification of parameters relating to the fractures intersecting canisters and the earthquake rupture. Each earthquake is represented as an instantaneous displacement on a plane represented by a rectangle. La Pointe *et al*. (1997) used Poly3D to estimate the effects of an earthquake in terms of displacements on fractures that intersect canister holes in a repository. The study was based on the geology of the Äspö area. Poly3D parameter values were provided. Subsequently, La Pointe *et al*. (1999) undertook similar analyses using Poly3D for the Aberg, Beberg, and Ceberg generic sites. La Pointe *et al*. (1999) used the discrete fracture network code FRACMAN to generate fractures that intersect canister holes as input to the Poly3D calculations.

3.8.3 Code Verification and Validation

The Stanford University website claims that many different aspects of Poly3D have been verified by comparisons with analytical solutions from elasticity theory, and notes that the process of verification is on-going and will be enhanced by increasing the number of users. The code has been applied to a wide variety of academic and industry problems.

La Pointe *et al*. (1997) presented two test cases for Poly3D. One case involved comparison of a Poly3D result with an analytical solution for displacement along a line in an infinite medium for a plane strain problem. Parameter values were provided for the test case. Details of the analytical solution were not given, although a reference to the solution was given. The Poly3D solution showed good agreement with the analytical solution.

For the second case, displacements along two intersecting fractures in an infinite medium were considered. Poly3D calculations were performed for configurations involving single fractures and the two solutions were superposed. The superposed solution was compared to Poly3D solutions for a configuration involving both fractures. Good agreement demonstrated that Poly3D represents the principle of superposition correctly. Not all parameter values were provided in this case.

Information on the verification of the modified form of Poly3D that calculates the variation in displacement along a fracture (La Pointe *et al*., 1999) has not been identified.

Conservatisms in Poly3D were evaluated by LaPointe *et al*. (2000) by comparison with the fracture mechanics code FRANC3D. Fracture propagation, interaction between fractures, and fracture friction and cohesion are not included in Poly3D, but these processes were shown to reduce the potential for slip on fractures.

3.8.4 Summary

The Poly3D model was developed at Stanford University to evaluate stress and strain development along faults and fractures. SKB has used Poly3D for studying the effects of fracture displacements on the integrity of canisters in disposal holes. No comprehensive description of the model has been identified, although such information is likely to be available from Stanford University.

The code has been verified at Stanford University, and SKB has undertaken verification studies involving comparison of Poly3D results with analytical solutions. Information on the verification of the modified form of the code to solve for variation in displacement along a fracture has not been identified.

3.9 UDEC, 3DEC, FLAC, and FLAC3D

UDEC (Universal Distinct Element Code), 3DEC (a three-dimensional version of UDEC), FLAC (Fast Lagrangian Analysis of Continua) and FLAC3D (a three-dimensional version of FLAC) are geotechnical modelling codes produced by HCItasca. Information on each of these codes can be found at HCItasca's website www.itascacg.com. These codes have been used by SKB over many years in studies of the thermo-hydro-mechanical behaviour of repository host rock. Examples of code usage include:

UDEC — Used by Hökmark (1990) to analyse the behaviour of fractured rock in the near field of a repository based on conditions in the Stripa mine. Used by Hakami *et al*. (1998) to determine equivalent material properties for the repository region for use in a 3DEC modelling study of thermo-mechanical effects. Used by Hakami and Olofsson (2002) in an analysis of shear displacement on pre-existing fractures located in the repository area resulting from thermal loading.

3DEC — Used by Hökmark and Israelsson (1991) in simulations of the behaviour of the jointed rock mass in the near field of a KBS3-type tunnel and deposition hole based on conditions in the Stripa mine. Used by Hakami *et al*. (1998) to study thermo-mechanical effects in a KBS-3-type repository.

FLAC — Used by Pusch and Hökmark (1992) in a study of rock creep in the repository near field. Used by Hökmark (1994) to evaluate rock mechanics and fluid flow in a tunnel plug design study. Used by Hökmark and Fälth (2003) in a thermal analysis of the repository near field.

FLAC3D Used by Hakami and Olofsson (2000) to investigate how the rock mass in the near field of a KBS-3-type repository will be affected by excavation of tunnels and deposition holes and the thermal load from the deposited waste. Used by Hakami and Olofsson (2002) in a three-dimensional analysis of shear displacements on a pre-existing fracture located in the repository area resulting from thermal loading.

3.9.1 Code Description

Descriptions of the main features of UDEC, 3DEC, FLAC, and FLAC3D are available on the HCItasca website.

In both UDEC and 3DEC the modelling domain is divided into joints and rock blocks. Using the distinct element method, the rock blocks are divided into triangular (2D) or tetrahedral (3D) zones. Interactions between the rock blocks depend on the mechanical properties of the joints between the blocks. Hökmark and Israelsson (1991) outlined the material models, boundary conditions, and thermal and flow logic in UDEC and 3DEC. Key features are:

- Linearly-elastic and Mohr-Coulomb elastic/plastic models for the intact rock.
- A Mohr-Coulomb friction model and a linearly-elastic stress-closure relation for joint normal displacements. A continuously yielding model is also available in UDEC.
- A finite difference solution to the thermal diffusion equation in UDEC. Heat transfer is calculated using analytically derived point source fields in 3DEC.
- Calculation of stresses induced by thermal expansion.
- Fluid flow in fractures in UDEC including calculation of the effects of fluid pressure on fracture aperture.

Johansson *et al*. (1991) provided details of the equations and the explicit central difference scheme used in UDEC and 3DEC to determine displacements and forces in a study of the mechanical response to a repository in Finnish bedrock.

FLAC and FLAC3D assume the rock behaves as a continuum, although it is possible to model a limited number of discontinuities in FLAC3D. The codes may be used to model the mechanical behaviour of a densely fractured crystalline rock mass using equivalent continuum material properties. Heat transfer, creep, and fluid flow may be modelled. The codes use explicit finite difference solution schemes.

3.9.2 Code Usage

No information on running UDEC, 3DEC, FLAC, or FLAC3D has been obtained under this project, although user's guides are available via the HCItasca website.

SKB's applications of UDEC, 3DEC, FLAC, and FLAC3D provide some insights into key issues and assumptions in code usage. For example, Hökmark and Israelsson (1991) demonstrated the importance of undertaking three-dimensional calculations in determining the behaviour of fractures around openings based on a comparison of the 3DEC results with UDEC results.

Hakami *et al*. (1998) provided an example of the use of 3DEC in modelling the mechanical influence of major fault zones on a repository. The analysis involved implementing a fine discretization close to the repository, with coarser gridding in the outer regions. A Mohr-Coulomb plasticity model was used for the intact rock blocks, with an elastic-plastic constitutive model with Coulomb slip failure for the fracture zones. UDEC was used to determine equivalent material properties for the repository region for use in the 3DEC modelling.

In a FLAC 3D study of the repository nearfield undertaken by Hakami and Olofsson (2000), the rock mass was modelled as a homogeneous and isotropic elasto-plastic continuum. The effective stress concept was used with a Mohr-Coulomb yield criterion. The modelling sequence to determine the stress field encompassed excavation of the repository tunnel, excavation of deposition holes, introduction of groundwater pressure, and calculation of thermal response at selected times. Thermal calculations were performed using a large model and thermo-mechanical calculations were performed at selected times in a smaller model. The model was simplified by assuming planes of symmetry between parallel tunnels and between deposition holes.

3.9.3 Code Verification and Validation

No information on the verification or validation of UDEC, 3DEC, FLAC, or FLAC3D has been obtained under this project. However, verification problems are available via the HCItasca website.

The extensive use of these codes internationally over many years engenders a high level of confidence that they are tried and tested. UDEC was first released in 1985, FLAC was released in 1986, 3DEC in 1988, and FLAC3D in 1994, and the HCItasca website claims a user-base that includes over 5000 licenses of HCItasca codes located in more than 42 countries.

3.9.4 Summary

UDEC, 3DEC, FLAC, and FLAC3D are produced by HCItasca, and have been used by SKB over many years in studies of the thermo-hydro-mechanical behaviour of repository host rock. Although the modelling studies presented by SKB generally do not describe the details of the processes modelled and the solution techniques used, and do not include verification studies, this information would be available from

HCItasca. The codes have had a broad user base for many years and may be considered to be fit-for-purpose with a high level of confidence.

3.10 M3

The Multivariate Mixing and Mass balance model (M3) was developed by SKB (Laaksoharju *et al*., 1999a; 1999b) to study the evolution of groundwater composition. M3 evaluates geochemical reactions between the groundwater and the minerals it contacts, and the mixing of groundwater types of different origins.

M3 has been used to study hydrochemical conditions at Aberg, Beberg and Ceberg (Laaksoharju *et al*., 1998; SKB, 1999a) and at the Äspö Hard Rock Laboratory (Laaksoharju *et al*., 1999c). SKB plans to use the M3 model to calculate mixing proportions of different groundwater types for a KBS-3 repository concept (SKB, 2003)

3.10.1 Code Description

M3 is a mathematical model for comparing the properties of different groundwater samples and drawing conclusions on the evolution of the groundwater. The model has three stages summarised by Laaksoharju *et al*. (1999a; 1999b):

1. Identify waters of different origins. A multivariate statistical technique, Principal Component Analysis (PCA), is used to cluster the groundwater data and construct an ideal mixing model with specific chemical components and isotopes. Each principal component is an equation of linear combinations of these chemical components and isotopes that aims to describe the information in the groundwater data. Reference waters and end-member waters are identified, which are the compositions used to compare with samples.

2. Infer the mixing ratio of the reference waters to reproduce the chemistry of groundwater samples.

3. Identify any deviations between the chemical measurements of each sample and the theoretical chemistry from the mixing calculation, which are interpreted as resulting from interactions with the solid minerals. Mass balance calculations are used to define the sources and sinks for different elements. The evolution of the groundwater can then be described.

The principal reference for M3 is Laaksoharju *et al*. (1999b), which provides a detailed description of the M3 model and several references to PCA theory. However, details of how PCA has been applied in the M3 model have not been given. Laaksoharju *et al*. (1999a; 1999b) do present an equation for calculating the mixing proportions of reference waters that contribute to a particular observation.

3.10.2 Code Usage

Laaksoharju *et al*. (1999b) explain that M3 is run as a toolbox under MATLAB, and provides information on installation of M3. A detailed description of how to run M3, with helpful images of screen menus, is also provided, and an example application is presented.

Laaksoharju *et al*. (1999a; 1999b) provided M3 modelling procedures and rules and limitations on its use and, in particular, identified:

- the importance of selecting appropriate reference waters; and
- the importance of being able to summarise more than 60% of the variability in the groundwater data set with the first and second principal components (linear combinations of ten variables that describe the majority of groundwaters) for the M3 approach to work.

3.10.3 Code Verification and Validation

Laaksoharju *et al*. (1999a) reported that M3 has been successfully tested against the reaction path model NETPATH in an analysis of a specific groundwater at the fracture zone scale. Laaksoharju *et al*. (1999a) cited Banwart *et al*. (1995) for this code comparison, but the latter report has not been obtained under this project.

The accuracy of the mixing calculations was tested using a back propagation test. Mixing calculations were performed on groundwater samples of known mixing proportions (Laaksoharju *et al*., 1999a). The error was found to be ±10.45% at 90% confidence for Äspö data.

The ability of M3 to predict the contents of conservative groundwater tracers at Äspö was compared with the results of traditional mixing models. M3 was generally found to give smaller errors. Tests were also performed using Äspö site data in which the number, type and composition of reference waters were varied in order to find the model that gave the lowest deviation for conservative water constituents (Laaksoharju and Wallin, 1997).

Gurban *et al*. (1998) and Gurban *et al*. (1999) evaluated uranium transport around the Oklo reactor zones at Bangombé and Okelobondo, respectively, using M3 and the solute transport and chemical speciation code HYTEC. The results of the codes were found to be in reasonable agreement.

Laaksoharju *et al*. (2000) found that the occurrence and the distribution of water types and the mass-balance calculations for carbonate were in general agreement with previous interpretations of groundwater composition and modelling of the Whiteshell Research Area in Canada.

3.10.4 Summary

The M3 model was developed by SKB to study the evolution of groundwater composition.

Laaksoharju *et al*. (1999b) provide a comprehensive description of how to run M3. However, no details of the implementation of Principal Component Analysis (PCA) theory and the mass balance calculation method have been identified in any of the references reviewed under this project.

M3 has been tested successfully against a reaction path model, a speciation code, previous interpretations of groundwater chemistries, and in back propagation testing.

4 Software Quality Assurance

This section presents a brief review of approaches to software quality assurance (QA) adopted in the nuclear industry. Software QA standards are discussed and the application of QA standards to software used in nuclear facilities and various radioactive waste management projects is summarised. Requirements on testing and documenting code are highlighted.

4.1 Software QA Standards for Nuclear Safety Applications

Maul *et al*. (1999) reviewed QA issues in repository performance assessments on behalf of SKI, and DOE (2003a) reviewed QA standards for safety software in US Department of Energy (DOE) nuclear facilities. These reviews considered ISO (the International Organisation for Standardisation) requirements and ASME (American Society of Mechanical Engineers) standards, as well as other international standards for quality and software, including those prepared by the International Atomic Energy Agency (IAEA) and the International Electrotechnical Commission (IEC). This section considers the key ISO and ASME standards.

4.1.1 ISO 9001-2000

The ISO quality management systems requirements in the current standard, ISO 9001-2000, do not specifically address computer software. An earlier version of the standard, ISO 9001 (1994), was accompanied by guidance on its application to software in the standard, ISO 9000-3, and Maul *et al*. (1999) recommended that software development should adhere to ISO 9000-3 where applicable, although the guide was not focused on nuclear safety. DOE (2003a) considered that supplementary requirements would be needed to apply ISO 9001-2000 to nuclear safety applications.

Guidelines are available for the application of ISO 9001-2000 to software development under the TickIT scheme (www.tickit.org). The TickIT scheme provides guidance on defining and implementing a quality system that covers all processes in the software life-cycle within the framework of ISO 9001-2000. A successful audit by a TickIT-accredited certification body results in the award of a certificate of compliance to ISO 9001-2000, endorsed with a TickIT logo. TickIT is supported by the Swedish and UK software industries.

4.1.2 ASME NQA-1-2000

The ASME standard NQA-1-2000 (Quality Assurance Requirements for Nuclear Facility Applications) represents the most comprehensive nuclear QA programme standard for application to safety software. NQA-1-2000 has resulted from the merging of three NQA standards: NQA-1 (Quality Assurance Program Requirements for Nuclear Power Plants), NQA-2 (Quality Assurance Requirements for Nuclear Power Plants), and NQA-3 (Quality Assurance Requirements for the Collection of Scientific and Technical Information for Site Characterization of High-Level Nuclear

Waste Repositories). Maul *et al*. (1999) had previously recommended that consideration be given to the ASME standard NQA-3, because it is directly applicable to repository performance assessments.

Key quality requirements of NQA-1-2000 are defined in Subpart 2.7 (Quality Assurance Requirements for Computer Software for Nuclear Facility Applications). DOE (2003a) summarised the key elements of the software QA process addressed by NQA-1-2000 as:

- management;
- design;
- reviews;
- verification;
- testing;
- documentation and records;
- software engineering method;
- problem reporting and corrective action;
- configuration management;
- acquisition/procurement;
- operation;
- maintenance;
- retirement.

NQA-1-2000 supports a graded approach to QA in that all or part of the standard may be applied for specific software projects depending on the nature and importance of the work or service.

4.2 Safety Software QA in US DOE Nuclear Facilities

Recently, the US DOE has made significant efforts to ensure that software quality assurance (SQA) issues are addressed at DOE nuclear sites. The DOE's SQA activities represent a response to a review and recommendations by the US Defense Nuclear Facilities Safety Board on safety-related computer codes used by the DOE at defence nuclear facilities. Key findings of the review board included:

- inappropriate use of software;
- inconsistent SQA across facilities;
- variability in guidance and training;
- concerns over software quality; and
- concerns over the proficiency of personnel using software.

Approaches to addressing these SQA issues have been presented for two classes of safety-related software:

- DOE (2003b) described a plan and criteria for SQA evaluation of toolbox codes and determined actions required for codes to meet SQA standards. Toolbox codes are codes widely used by the DOE for safety analysis applications or codes that could have significant consequences in the event of failure.

- DOE (2004a) addressed SQA issues for other safety-related design codes used at DOE facilities, but developed and maintained externally to the DOE.

SQA issues for different categories of code are discussed in the following sub-sections.

4.2.1 Toolbox Codes

DOE (2003b) presented SQA evaluation criteria for toolbox codes aimed at satisfying:

- 10 CFR 830 (Nuclear Safety Management) Subpart A (Quality Assurance Rule).

- ASME NQA-1-2000 (principally Subpart 2.7 - Quality Assurance Requirements for Computer Software for Nuclear Facility Applications).

Procedures for implementation of the NQA-1-2000 requirements were derived based on review of procedures for meeting NQA-1 requirements at Sandia National Laboratories, the Savannah River Site, and the Yucca Mountain Project. The following list of requirements was identified:

1. Software Classification
2. SQA Procedures/Plans
3. Dedication
4. Evaluation
5. Requirements
6. Design
7. Implementation
8. Testing
9. User Instructions
10. Acceptance Test
11. Operation and Maintenance
12. Configuration Control
13. Error Impact
14. Access Control

Details of these requirements are presented in DOE (2003b) and the SQA plan has been summarised by O'Kula and Eng (2004). Some of these steps are graded in that their requirements depend on whether the code is under development, exists but did not follow NQA-1-2000 or similar primary criteria, or has been purchased.

Several formal documents are required to demonstrate compliance with the requirements:

- Software Quality Assurance Plan;
- Software Requirements Document;
- Software Design Document;
- Test Case Description and Report;
- Software Configuration and Control Document;
- Error Notification and Corrective Action Report; and
- User's Instructions (alternatively, a user's manual).

The toolbox safety analysis codes are thus supplemented with DOE-published user guidance documents that establish the applicable usage, appropriate range of use, and cautionary instructions to minimise the potential for inappropriate software applications. The DOE maintains, manages, and distributes toolbox codes via a central source.

4.2.2 Safety-Related Design Software

DOE (2004a) considered SQA issues for safety-related design software and general analytical software used at DOE nuclear facilities, but not designated as toolbox codes. A survey of such software was undertaken and many codes were identified that are widely used outside the DOE, most of which can be considered to have widespread acceptance and have extensive user's groups. DOE (2004a) tabulated information on these codes, including the area of applicability, code function, software developer, SQA standards cited, training, and number of users. An example of safety-related design software relevant to the present code documentation and testing project is the ABAQUS geotechnical code.

DOE (2004a) noted that the software listed tends to be industry-independent, typically spanning many sectors of engineering design, and concluded that, because the software is typically proprietary, commercial interests create a need for the software developer to identify and correct deficiencies or errors in a timely manner. This aspect of code management is reflected in the proposed DOE SQA programme for such codes, which assumes that the developer has an adequate process to verify, test, and control the software prior to its release. However, DOE (2004a) recommended setting minimum requirements for QA standards for theses codes, such as NQA-1 or ISO 9000.

The proposed DOE programme requires other aspects of the SQA process to be present in application of these codes. The DOE must ensure:

- adequate user training;
- reporting and tracking of errors and deficiencies; and
- incorporation of lessons learned.

The approach requires that each code user must identify and justify the version of software, understand the limitations of the software, use inputs and assumptions that are consistent with the intent of the software and the specific application, and obtain sufficient peer review of their analyses.

The DOE (2004a) code survey designated some software as "analytical". Analytical software does not focus on any specific application, and is widely used outside the DOE. It is usually general-purpose, proprietary software used to solve a wide array of problems in design as well as other engineering areas (e.g., MATLAB and Excel). Such software has been in use for many years and has even greater acceptance and a more extensive user base than safety-related design software. Commercial interests would be expected to ensure that a SQA process exists.

The level of detail and documentation required to ensure software quality is graded based on the level of model complexity. DOE (2004a) noted that simple models or mathematical manipulations that are appropriately documented may be checked easily by hand calculations or with a calculator. However, the development of more complex models using analytical software can be equivalent to designing independent software and, as such, would be subject to all the requirements that would be called for by generation of any propriety code, including independent review.

The safety-related design software and analytical software are typically used at more than one DOE facility and, thus, DOE (2004a) proposed a web-based information system for error reporting and tracking, and to share information on code usage.

4.3 QA for Repository Performance Assessment Software

Software quality assurance has been addressed rigorously in many radioactive waste disposal projects. The following sub-sections discuss SQA related to performance assessments for the Yucca Mountain Project in the US, performance assessment software developed by Sandia National Laboratories in the US, and performance assessment software applied by BNFL to the Drigg low-level waste disposal facility in the UK.

4.3.1 Software QA Requirements for the Yucca Mountain Project

The Quality Assurance Requirements and Description (QARD) is the principal Quality Assurance (QA) document for the Yucca Mountain Project in the US (DOE, 2004b). The QARD establishes the minimum requirements for the QA programme designed to meet the QA requirements for the disposal of high-level radioactive wastes in geologic repositories (10 CFR 60, Subpart G[1]). In addition to regulatory documents, the QARD requirements are derived from industry documents, such as the ASME standards NQA-1 and NQA-2 for nuclear facilities, and NQA-3 for waste repositories (See Section 4.1.2).

The QARD includes a supplement (Supplement I Software) that establishes requirements for the acquisition, development, modification, control, and use of software in a rigorous graded approach based on a software life-cycle methodology.

[1] 10 CFR 60, Subpart G imposes on geologic repositories for high-level waste the applicable requirements of the QA criteria for nuclear power plants and fuel reprocessing plants (10 CFR 50, Appendix B).

The detailed requirements of the software QA process are presented in DOE (2004b) for the following key components:

- Software Planning.

- Software Life-Cycle Requirements:
  - Requirements Phase;
  - Design Phase;
  - Implementation Phase;
  - Testing Phase;
  - Operations and Maintenance Phase;
  - Installation and Checkout Phase;
  - Retirement Phase.

- Software Configuration Management:
  - Configuration identification;
  - Configuration change control;
  - Configuration status accounting.

- Defect Reporting and Resolution.

- Software Procurement.

- Software Previously Developed Not Using this Supplement.

- Control of the Use of Software.

The number of life-cycle phases and the relative emphasis placed on each phase of the software life-cycle will depend on the nature and complexity of the software. Software life-cycle activities may be performed in an iterative or sequential manner.

DOE (2004b) requires that, as far as possible, software verification and validation is carried out by individuals not associated with the development of the software.

Documentation requirements should be set out in the software plan, and should include the following key aspects:
- Design;
- User information;
- Validation;
- Software modifications.

There are limited requirements on software routines and macros that have been developed using software such as compilers, word processors, spreadsheets, and database managers and that can be independently verified by inspection or hand calculation. These limited requirements cover software identification, and documentation of inputs, generated results, algorithms, and verification results.

Software procured or previously developed requires software planning and a software life-cycle, excluding the design phase and the code development part of the implementation phase. However, individuals or organisations developing and supplying software should have policies and procedures that meet the requirements set out in DOE (2004b). Required documentation should be delivered or made available and the purchaser should assume responsibility for the applicable requirements.

Software developed prior to DOE (2004b) should be placed under configuration controls. The user organisation should first identify activities and documents required in order for the software to be placed under configuration controls (e.g., application requirements, test plans and case, user documentation, independent review, and approval).

4.3.2 Software QA for the SNL Nuclear Waste Management Programme

The processes used to qualify or control software in the nuclear waste management programme at Sandia National Laboratories (SNL) in the US are presented in Procedure NP 19-1 (SNL, 2000). The application of requirements is determined by the intended use of the software output. The most rigorous requirements (life-cycle management) are applied to software that is used to demonstrate compliance with disposal regulations or whose output is relied upon to make design, analytical, operational, or compliance-based decisions with respect to waste confinement processes. SNL (2000) listed the following examples of such compliance decision software:

- software used to assess site performance;
- software used to analyse data for, or produce input to, a performance assessment calculation; and
- software used to collect data.

The life-cycle process comprises the following eight phases:

- Transition;
- Requirements;
- Design;
- Implementation;
- Validation;
- Installation and checkout;
- Maintenance; and
- Retirement.

The transition phase is specifically for existing software and the design phase for developed software. The life-cycle process requires numerous records including:

- Requirements Document;
- Verification and Validation Plan;
- Design Document;
- Implementation Document;
- User's Manual;
- Validation Document.

Software used to make programmatic decisions, such as scoping or screening analyses to develop, implement, or test potential improvements to existing methodologies do not fall under the life-cycle process. Instead, the following are required:

- Software Name;
- Software Version;
- Platform;
- Functionality;
- Reasonable Results;
- Test Cases.

Other information relating to the system configuration and the use of the software should be provided.

SNL (2000) noted that spreadsheets and graphing programs, the results of which are verifiable by hand calculations, and systems software are exempt from QA procedure NP 19-1.

4.3.3 Software QA for the BNFL 2002 Drigg Post-Closure Safety Case

BNFL's QA system for the 2002 Drigg Post-Closure Safety Case (PCSC) is set out in BNFL (2002a). The overall approach to QA adopted by BNFL follows international standards (including ISO 9001-2000 and IAEA standards), BNFL company policies, BNFL facility management systems, and project-specific QA plans. BNFL technical services are provided as Research & Technology (R&T) projects, which are subject to a QA system termed the R&T Integrated Management System (RIMS).

The 2002 Drigg PCSC was carried out as an R&T project termed the Drigg Technical Programme (DTP), which was subject to RIMS as well as a number of DTP-specific QA requirements. RIMS includes several procedures for environmental model development and management. The software tools and codes report, BNFL (2002b), describes the quality assurance process for the development and use of codes in the Drigg PCSC. This quality assurance process is consistent with the requirements of RIMS and the DTP procedures.

Software development under the DTP followed a life-cycle methodology with the following phases:

- Project initiation;
- Scoping phase;
- Functional design phase;
- Architectural design phase;
- Sub-program design phase;
- Sub-program coding;
- Sub-program testing;
- Integrated program testing;
- Project completion.

The software QA standards require nine detailed code documents:

- User Requirements Document;
- Development Plan;
- Functional Specification;
- Architectural Design Specification;
- A Sub-program Description Document;
- Sub-program Test Log;
- Program User's Guide;
- Program Programmer's Guide;
- Program Verification Report.

The major codes used to support the 2002 Drigg Post-Closure Radiological Safety Assessment (PCRSA) within the PCSC were developed internally by BNFL and have been subject to the above mentioned QA regime.

Simple codes, such as pre- and post-processing codes developed internally to support the PCRSA, are subject to a reduced version of the software cycle. These codes are typically of the order of up to a hundred lines of code, with no complicated calculations or procedures. The code is documented on calculation sheets, and testing involves checking input cases and visual checking.

BNFL has specific procedures for internal installation and use of external codes. These procedures require that, prior to acquisition of the software, the purchase is justified through consideration of code requirements and capabilities. The code is then appraised before approval for use. An installation test plan is formulated that includes any supplier's tests and any other tests deemed necessary to ensure verification and suitability of the code. This process must be fully documented. A similar exercise is undertaken for codes developed and used externally to BNFL, whereby the QA procedures used by external contractors for installation, running and control of the code are assessed for appropriateness against BNFL procedures. BNFL (2002b) includes a discussion of the QA status for each external code used in the 2002 Drigg PCSC.

A separate QA approach involving standard installation and testing is adopted for readily available commercial software, such as software used to support data interpretations and standard word processor, spreadsheet, and database software. Full checking procedures are used for any work produced using these codes, including calculations performed, and work produced externally.

4.4 Summary

The quality management systems requirements in the standard, ISO 9001-2000, do not specifically address computer software, although guidelines are available for the application of ISO 9001-2000 to software development under the TickIT scheme. The ASME standard NQA-1-2000 is the most comprehensive QA programme for software used in nuclear facilities. The standard supports a graded approach to QA in that all or part of the standard may be applied for specific software projects depending on the nature and importance of the analysis.

NQA-1-2000 (or its predecessors) has been adopted at US DOE nuclear facilities and radioactive waste management projects, and an approach that appears consistent with NQA-1-2000 has been adopted by BNFL for the assessment of the low-level radioactive waste disposal facility at Drigg in the UK. These projects require the acquisition, development, modification, control, and use of software in a rigorous graded approach based on a software life-cycle methodology. In each case, the software QA process broadly covers:

- Software planning;
- Software life-cycle;
- Software configuration management;
- Defect reporting and resolution;
- Software procurement;
- Control of the use of software.

Documentation requirements of the life-cycle process typically include:

- Requirements Document;
- Verification and Validation Plan;
- Design Document;
- Implementation Document;
- User's Manual;
- Validation Document.

BNFL used a software life-cycle approach for the major codes used in developing the 2002 Drigg PCRSA. SNL noted that the most rigorous requirements (life-cycle management) are applied to software that is used to demonstrate compliance with disposal regulations or is relied upon in key decision-making on waste confinement processes.

BNFL has specific procedures for internal installation and use of external codes that include a phase of code appraisal. For codes developed and used externally to BNFL, the QA procedures used by external contractors for installation, running and control of the code are assessed for appropriateness against BNFL procedures. A similar approach is taken at the Yucca Mountain Project. Also, the US DOE requires that software developed prior to establishment of its QA procedures is placed under configuration controls.

Consistent with the graded approach, the waste management projects generally adopt a reduced version of the software cycle for simple codes, such as pre- and post-processing codes, and software developed using word processors, spreadsheets, and database managers that can be independently verified by inspection or hand calculation. These requirements generally cover software identification, and documentation of a range of inputs and generated results, algorithms, and verification results.

5 Summary and Conclusions

5.1 Summary

SKB is in the process of developing the SR-Can safety assessment for a KBS 3 repository. The assessment will be based on quantitative analyses using a range of computational codes aimed at developing an understanding of how the repository system will evolve. Clear and comprehensive code documentation and testing will engender confidence in the results of the safety assessment calculations.

This report presents the results of a review undertaken on behalf of SKI aimed at providing an understanding of how codes used in the SR 97 safety assessment and those planned for use in the SR-Can safety assessment have been documented and tested. Having identified the codes used by SKB, several codes were selected for more detailed review. Consideration was given not only to codes used directly in SKB's safety assessment calculations, but also to some of the less visible codes that are important in quantifying the different repository barrier safety functions. SKB's documentation and testing of the following codes were reviewed:

- COMP23 - a near-field radionuclide transport model developed by SKB for use in safety assessment calculations.
- FARF31 - a far-field radionuclide transport model developed by SKB for use in safety assessment calculations.
- PROPER - SKB's harness for executing probabilistic radionuclide transport calculations using COMP23 and FARF31.
- The integrated analytical radionuclide transport model that SKB has developed to run in parallel with COMP23 and FARF31.
- CONNECTFLOW - a discrete fracture network model/continuum model developed by Serco Assurance (based on the coupling of NAMMU and NAPSAC), which SKB is using to combine hydrogeological modelling on the site and regional scales in place of the HYDRASTAR code.
- DarcyTools - a discrete fracture network model coupled to a continuum model, recently developed by SKB for hydrogeological modelling, also in place of HYDRASTAR.
- ABAQUS - a finite element material model developed by ABAQUS, Inc, which is used by SKB to model repository buffer evolution.
- Poly3D - a displacement discontinuity model developed at Stanford University and used by SKB to study the effects of movement on fractures that intersect canister deposition holes.

- UDEC, 3DEC, FLAC, and FLAC3D - geotechnical models developed by HCItasca, and used by SKB in thermo-hydro-mechanical analysis of repository host rock.

- M3 - a multivariate mixing and mass balance model developed by SKB to study the evolution of groundwater composition.

Summary information on the commercially available codes (CONNECTFLOW, ABAQUS, Poly3D, UDEC, 3DEC, FLAC, and FLAC3D) has been obtained from the developers' websites. The apparent extensive testing and broad usage of these codes offers a high level of confidence that they are fit for intended purpose. ABAQUS, in particular, has had a worldwide user base for over 20 years and, although CONNECTFLOW has been developed recently, its two component models, NAPSAC and NAMMU, have been in wide use for over 10 years. Poly3D has had fairly extensive research usage since the mid-1990s and its development has had industrial support in recent years. UDEC, 3DEC, FLAC, and FLAC3D were all first released over ten years ago, and have been used extensively worldwide.

SKB appears to have modified or developed a number of commercial codes in-house. For example, a temperature-driven water vapour flow code and a mechanical model of a clay buffer have been developed for use with ABAQUS, and a code to solve for variation in displacement along a fracture has been developed for Poly3D. It is unclear whether these developments have become an integral part of, and have been subject to similar levels of testing as, the main code.

Varying standards of code documentation have been identified for the SKB codes COMP23, FARF31, PROPER, the analytical radionuclide transport code, DarcyTools, and M3. The recent DarcyTools reports are of a high standard, providing comprehensive information on the model basis, code usage, and code verification and validation. SKB acknowledges that the DarcyTools code requires further application to build confidence in its usage, and that a high level of expertise in the code and Fortran programming would be required if some of the more advanced features were to be used.

The COMP23 documentation is less comprehensive. In particular, details of the analytical methods that may be selected when fine solutions are required have not been included in the user's guide (although a recently released version of the COMP23 user's guide has not been checked for such information under this project). Also, no single COMP23 verification report has been identified, although some components of COMP23 have been tested in various code comparison studies. SKB (2004) noted that a COMP23 validation report will be produced. A user's guide and a model validation and verification document have been produced for FARF31, although the user's guide is an SKB progress report that is not available via the SKB website. A user's guide is available for PROPER, but it does not include detailed information on using PROPER in repository safety assessments. Information on testing PROPER has not been identified.

Details of the analytical transport model have been provided in a paper published in the Nuclear Technology journal. However, SKB does not appear to have produced a user guide and verification report for the model, although a verification exercise was presented in the Nuclear Technology paper.

An M3 user guide has been produced, although full details of the M3 solution method have not been identified. An M3 verification and validation report has not been identified under this project, although various reports and papers on M3 testing have are available.

To develop a greater understanding of software documentation and testing standards, a brief review has been undertaken of software QA requirements in other radioactive waste management programmes. In general, the projects studied require that software is managed under a rigorous graded approach based on a software life-cycle methodology, with documentation requirements that include user's manuals and verification and validation documents. These requirements also include procedures for the use of external codes.

Consistent with the graded approach, the waste management projects generally adopt reduced version of the software cycle for simple codes, such as pre- and post-processing codes, and software developed using word processors, spreadsheets, and database managers that can be independently verified by inspection or hand calculation.

5.2 Conclusions

Varying standards of code documentation have been identified for the SKB codes considered in this project. User's guides and verification reports should be developed for all of SKB's codes that are of a similar standard to the DarcyTools documents and are consistent with appropriate software quality assurance (QA) procedures.

Review of software QA requirements in other radioactive waste management programmes has provided a useful insight into the rigorous graded software life-cycle methodologies that are generally adopted in such programmes. In particular, the review has provided insights into the type of code documentation that might be expected to accompany the submission of a repository safety assessment. SKB should provide details of its software QA procedures covering different categories of software (e.g., internal, commercial, academic, and simple codes).

In order to gain greater understanding and confidence in, and become more familiar with SKB's codes, SKI could consider testing some of SKB's codes against its own codes. This would also serve as a useful background to any future sensitivity analyses that SKI might conduct with these codes. Further, SKI could review its own software QA procedures and the required extent of documentation and testing of its own codes.

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APPENDIX A

Codes used by SKB

A Introduction

Table A.1 provides information on the codes used directly and indirectly in the SR 97 safety assessment (SKB, 1999a and b), and codes that SKB plans to use in the SR-Can safety assessment that are additional to, or alternative to, the codes used in SR 97 (SKB, 2003; SKB 2004).

The findings have been organised in Table A.1 according to the scenario-based structure used to present the SR 97 assessment:
- initial state;
- base scenario;
- canister defect scenario;
- climate scenario;
- tectonics - earthquake scenario; and
- scenarios based on human actions.

Within this structure, the codes have been presented in terms of the following processes (where applicable):
- radiation-related;
- thermal evolution;
- hydraulic evolution;
- mechanical evolution;
- chemical evolution; and
- radionuclide transport.

Table A.1 contains information on the code used in each part of the assessment or supporting studies, a brief statement on the code’s function, and references to its usage identified in the SR 97 reports (SKB, 1999a and b). In many places in the SR 97 reports, particularly with regard to analyses supporting the main assessment, code usage is implied but the code has not been identified. Where possible, the code has been identified by consulting the supporting references. In some cases the supporting references have not been obtained, in which case a question mark has been entered in the ‘code’ column.

Information on the codes that SKB plans to use in the SR-Can safety assessment that are additional or alternative to the codes used in SR 97 was extracted from the SR-Can planning report (SKB, 2003) and the SR-Can interim report (SKB, 2004). This information was added to a final column in Table A.1.

Table A.1 Codes used in the SR 97 safety assessment and planned for use in SR-Can safety assessment.

SR 97 safety assessment			SR-Can safety assessment
Code	**Function**	**References in SKB (1999a and b)**	**Additional/alternative codes/analysis referred to in SKB (2003; 2004)**
		Initial State	
?	Radionuclide inventory.	Håkansson, R., 1999. SKB R-99-74. (in Swedish)	
No code used	Instant release fraction of the inventory.	Johnson, L.H. and Tait, J.C., 1997. Release of segregated nuclides from spent fuel, SKB TR 97-18.	
?	Dose rate on the outside of the canister and buffer.	Håkansson, R., 1996. Studsvik Nuclear AB, NR-96/079. (in Swedish) Lundgren, K., 1997. ALARA Engineering Rapport 97-0028R. (in Swedish)	
?	Temperature on the surface of the fuel and canister.	Bjurström H., and Bruce, A., 1997. SKB PPM 97-3420-28. (in Swedish) Bjurström H., and Bruce, A., 1998. SKB PPM 98-3420-30. (in Swedish) Renström, P., 1997. Calculation of the fuel temperature in vacuous storage canisters made of copper with cast steel inserts. SKB PPM 97-3420-23.	
?	Thermo-mechanical finite element analysis of residual stresses in the lid weld.	Lindgren, L-E., Häggblad, Å., Josefson, L., and Karlsson, L., 1999. Thermo-mechanical FE-analysis of residual stresses and stress redistributions in butt welding of a copper canister for spent nuclear fuel. Int Conf on Structural Mechanics in Reactor Technology. SmiRT-15, Seoul, Korea, Aug 15-20.	
ANSYS	Canister spacing to meet the canister surface temperature limit.	Ageskog, L., and Jansson, P., 1999. Heat propagation in and around the deep repository. Thermal calculations applied to three hypothetical sites: Aberg, Beberg and Ceberg. SKB TR 99-02.	
?	Extent of excavation damage.	Andersson, P., 1994. SveBeFo Rapport 8. (in Swedish)	
UDEC	Simulated excavation (2D).	Hökmark, H., 1990. Distinct element method modelling of fracture behaviour in near-field rock. Stripa Project TR 91-01.	
3DEC	Simulated excavation (3D).	Hökmark, H. and Israelsson, J., 1991. Distinct element modelling of joint behavior in nearfield rock. Stripa Project TR 91-22.	

SR 97 safety assessment			SR-Can safety assessment
Code	**Function**	**References in SKB (1999a and b)**	**Additional/alternative codes/analysis referred to in SKB (2003; 2004)**
UDEC and 3DEC	Simulated excavation (Finnish bedrock).	Johansson, E., Hakala, M., and Lorig, L., 1991. Rock mechanical, thermomechanical and hydraulic behaviour of the near field for spent nuclear fuel. Report YJT-91-21. Nuclear Waste Commission of Finnish Power Companies, Helsingfors, Finland.	
?	Simulated excavation (SKI study).	Shen, B. and Stephansson, O., 1990. Modelling of rock mass response to repository excavations, thermal loading from radioactive waste and swelling pressure of buffer material. SKI Report 90:12.	
3DEC	3D near-field rock mechanics analysis (SKI study).	Shen, B. and Stephansson, O., 1996. SITE-94. Near-field rock mechanical modelling for nuclear waste disposal. SKI Report 96:17.	A geomechanical design model is planned (initial state), which is also to be used for analysis of thermal stress and load stresses.
?	3D continuum model of the stress state around a tunnel and deposition hole.	Johansson, E. and Hakala, M., 1995. Rock mechanical aspects on the critical depth for a KBS-3 type repository based on brittle rock strength criterion developed at URL in Canada. SKB AR D-95-014.	
FLAC	Model of creep deformation of a circular tunnel.	Pusch, R. and Hökmark, H., 1993. Mechanisms and consequences of creep in the nearfield rock of a KBS-3 repository. SKB TR 93-10.	Glamheden R, Hökmark H, Christiansson R, 2004. Modeling creep in jointed rock masses. Proc. 1st international UDEC/3DEC symposium, Bochum, Germany. Balkema. (In prep).
Base Scenario			
Radiation-related			
Excel	Fuel radioactivity and radiotoxicity with time (analytical) and dose rate outside the canister.	Hedin, A., 1997. Spent nuclear fuel - how dangerous is it? A report from the project “Description of risk”. SKB TR 97-13.	
Analytical solution	Heat generation with time (analytical).	Håkansson, R., 1999. SKB R-99-74. (in Swedish)	

SR 97 safety assessment			**SR-Can safety assessment**
Code	**Function**	**References in SKB (1999a and b)**	**Additional/alternative codes/analysis referred to in SKB (2003; 2004)**
Thermal			
ANSYS	Temperature in the buffer. Heat transfer in the geosphere with simplified near-field geometry.	Ageskog, L. and Jansson, P., 1999. Heat propagation in and around the deep repository. Thermal calculations applied to three hypothetical sites: Aberg, Beberg and Ceberg. SKB TR 99-02.	Hedin, A., 2003. Integrated System Evolution Model for an SNF Deep Repository. Proceedings from the 10th International High-Level Radioactive Waste Management Conference, Las Vegas 2003, American Nuclear Society (2003).
?	Temperature evolution (FEM study).	Thunvik, R. and Braester, C., 1991. Heat propagation from a radioactive waste repository. SKB 91 reference canister. SKB TR 91-16.	
Analytical solution	Temperature evolution (analytical solution).	Claesson, J. and Probert, T., 1996. Temperature field due to time dependent heat sources in a large rectangular grid. 1- Derivation of analytical solution. SKB TR 96-12.	
3DEC	Temperature evolution in the near field.	Hökmark, H., 1996. Canister positioning. Stage 1: Thermomechanical nearfield rock analysis. SKB AR D-96-014.	
STRES3D	Temperature evolution in the far field.	Israelsson, J., 1995. Global thermo-mechanical effects from a KBS-3 type repository. Phase 1: Elastic analysis. SKB PR D-95-008.	
?	Temperature effects of tunnel backfill.	Ageskog, L. and Jansson, P., 1998. Prototype repository. Finite element analyses of heat transfer and temperature-distribution in buffer and rock. SKB PR IIRL-98-20.	
Hydraulic			
PHOENICS	Large-scale flow and salinity model of Aberg.	Svensson, U., 1997. A regional analysis of groundwater flow and salinity distribution in the Äspö area. SKB TR 97-09.	
?	Large-scale flow and salinity model of Aberg.	Svensson, U., 1999. A numerical simulation of the origin and composition of the groundwater below Äspö. SKB R-99-39.	
NAMMU	Large-scale flow and salinity model of Beberg.	Hartley, L., Boghammar, A., and Grundfelt, B., 1998. Investigation of the large scale regional hydrogeological situation at Beberg. SKB TR-98-24.	

SR 97 safety assessment			SR-Can safety assessment
Code	**Function**	**References in SKB (1999a and b)**	**Additional/alternative codes/analysis referred to in SKB (2003; 2004)**
NAMMU	Large-scale flow and salinity model of Ceberg.	Boghammar, A., Grundfelt, B., and Hartley, L., 1997. Investigation of the large scale regional hydrogeological situation at Ceberg. SKB TR 97-21.	
ABAQUS	Temperature dependent saturation and swelling of the buffer.	Börgesson, L. and Hernelind, J., 1999. Coupled thermo-hydro-mechanical calculations of the water saturation phase of a KBS-3 deposition hole – Influence of hydraulic rock properties on the water saturation phase. SKB TR-99-41	Backfill saturation modelling using Code_Bright, a finite element code for thermo-hydro-mechanical analysis.
Mechanical			
?	Canister insert strength.	Ekberg, M., 1995. SKB PPM 95-3420-11. (in Swedish)	
“handbook” calculations	Effects of buffer swelling pressure on canister stress/strain.	Werme, L., 1998. Design premises for canister for spent nuclear fuel. SKB TR-98-08.	Karnland, O., Muurinen, A., and Karlsson, F., 2002. Bentonite swelling pressure in NaCl solutions - Experimentally determined data and model calculations. Submitted to: Applied Clay Science, 2002.
?	Effects of buffer swelling pressure on canister stress/strain.	Börgesson, L. and Hernelind, J., 1998. Uneven swelling pressure on the canister. FEM calculation of the effect of uneven water supply in the rock. SKB PPM 98-3420-33.	
?	Effects of rock movements on canister stress/strain.	Börgesson, L., 1992. Interaction between rock, bentonite buffer and canister. FEM calculations of some mechanical effects on the canister in different disposal concepts. SKB TR 92-30.	
?	Copper canister deformation.	Cakmak, E., 1994. SKB PPM 95-3420-01. (in Swedish)	
Analytical (in MATLAB)	Thermal stress analysis.	Probert, T. and Claesson, J., 1997. Thermoelastic stress due to a rectangular heat source in a semi-infinite medium. Application for the KBS-3 repository. SKB TR 97-26.	
STRES3D	Temperature evolution in the far field.	Israelsson, J., 1995. Global thermo-mechanical effects from a KBS-3 type repository. Phase 1: Elastic analysis. SKB PR D-95-008.	

SR 97 safety assessment			SR-Can safety assessment
Code	**Function**	**References in SKB (1999a and b)**	**Additional/alternative codes/analysis referred to in SKB (2003; 2004)**
3DEC	3D thermomechanical elastic calculations of stress around deposition holes.	Hökmark, H., 1996. Canister positioning. Stage 1: Thermomechanical nearfield rock analysis. SKB AR D-96-014.	Hökmark H, 2003. Canister positioning. Influence of fracture system on deposition hole stability. SKB R-03-19.
3DEC	Thermal stress-induced shear movements in the near field.	Shen, B. and Stephansson, O., 1996. SITE-94. Near-field rock mechanical modelling for nuclear waste disposal. SKI Report 96:17.	UDEC and FLAC3D: Hakami, E. and Olofsson, S-O., 2002. Numerical modelling of fracture displacement due to thermal load from a KBS 3 repository. SKB TR-02-08.
3DEC	Thermal stress-induced shear movements along fracture zones.	Hansson, H., Stephansson, O., and Shen, B., 1995. SITE-94. Far-field rock mechanics modelling for nuclear waste disposal. SKI Report 95:40. Israelsson, J., 1996. Global thermo-mechanical effects from a KBS-3 type repository. Phase 2: Three-dimensional modelling with major fracture zones – base case. SKB PR D-96-006.	
STRES3D and 3DEC	Thermal stress calculations.	Hakami, E., Olofsson, S-O., Hakami, H., and Israelsson, J., 1998. Global thermomechanical effects from a KBS-3 type repository. Summary Report. SKB TR-98-01.	
?	Rock creep-induced borehole deformations.	Eloranta, P., Simonen, A., and Johansson, E., 1992. Creep in crystalline rock with application to high level nuclear waste repository. Report YJT-92-10. Nuclear Waste Commission of Finnish Power Companies. Pusch, R., 1996. (in Swedish)	
ABAQUS	Material model with unsaturated water flow – finite element method.	Börgesson, L. and Johannesson, L-E., 1995. Thermo-hydro-mechanical modelling of water unsaturated buffer material. Status 1995. SKB AR 95-32. Hibbit, Karlsson and Sorensson. ABAQUS manuals. Börgesson, L. and Hernelind, J., 1995. DECOVALEX 1 – Test Case 3: Calculation of the Big Ben experiment – coupled modelling of the thermal, mechanical and hydraulic behaviour of water-unsaturated buffer material in a simulated deposition hole. SKB TR 95-29.	

SR 97 safety assessment			SR-Can safety assessment
Code	**Function**	**References in SKB (1999a and b)**	**Additional/alternative codes/analysis referred to in SKB (2003; 2004)**
		Börgesson, L. and Hernelind, J., 1997. THM modelling of a small scale wetting-heating test on compacted bentonite. CATSIUS CLAY PROJECT. Benchmark 2.2 SKB PR U-97-16. Alonso, E. and Alcoverro, J., 1997. CATSIUS CLAY – Calculation and testing of behaviour of unsaturated clay as a barrier in radioactive waste repositories (Stage 1: Verification exercises). EC Internal Report.	
ABAQUS	FEM study on the effects of swelling pressure.	Pusch, R. and Börgesson, L., 1992. PASS – Project on alternative systems study. Performance assessment of bentonite clay barrier in three repository concepts: DH. KBS-3 and VLH. SKB TR 92-40.	
ABAQUS	Canister movements in a deposition hole.	Börgesson, L., 1993. Study of the mechanical function of the buffer in the concept with two canisters in a KBS3 deposition hole. SKB AR 93-13.	
Chemical			
M3 (with WATEQ)	Mixing calculations to determine present-day hydrochemical conditions at Aberg, Beberg, and Ceberg. WATEQ for equilibrium calculations.	Laaksoharju, M., Gurban, I., and Skråman, C., 1998. Summary of hydrochemical conditions at Aberg, Beberg and Ceberg. SKB TR 98-03.	
M3	Mixing calculations.	Laaksoharju, M. and Wallin, B., 1997. Evolution of the groundwater chemistry at the Äspö Hard Rock Laboratory. Proceedings of the second Äspö International Geochemistry Workshop, June 6-7, 1995. SKB ICR 97-04.	
M3 (and HYTEC)	Mixing calculations, including comparisons with HYTEC.	Gurban, I., Laaksoharju, M., Ledoux, E., Madé, B., and Salignae, A.L., 1998. Indication of uranium transport around the reactor zone at Bangombé (Oklo). SKB TR-98-06.	

SR 97 safety assessment			SR-Can safety assessment
Code	**Function**	**References in SKB (1999a and b)**	**Additional/alternative codes/analysis referred to in SKB (2003; 2004)**
PHREEQC and ARASE	Geochemical effects of ice-sheet melting (equilibrium approach using PHREEQC and 2D non-equilibrium approach using ARASE).	Guimera, J., Duro, L., Jordana, S., and Bruno, J., 1999. Effects of ice melting and redox front migration in fractured rocks of low permeability. SKB TR-99-19.	
M3	Evolution of hydrochemical conditions at Aberg, Beberg, and Ceberg.	Rhén, I., Gustafson, G., Stanfors, R., and Wikberg, P., 1997. Äspö HRL – Geoscientific evaluation 1997/5. Models based on site characterisation 1986-1995. SKB TR 97-06.	
PHREEQC	Buffer ion-exchange model and evolution of pH and redox conditions.	Bruno, J., Arcos, D., and Duro, L., 1999. Processes and features affecting the near field hydrochemistry – groundwater-bentonite interaction. SKB TR-99-29.	PHREEQC: Near field geochemistry modelling: Domènech C, Arcos D, Bruno J, Karnland O, Muurinen A, 2004. Geochemical model of the granite-bentonite-groundwater at Äspö (Lot experiment) Mat. Res. Soc. Symp. Proc., 87: 855–860.
MIN_SURF	Ion exchange from sodium to calcium (using MIN_SURF - an extension of MINEQL).	Wanner, H., Wersin, P., and Sierro, N., 1992. Thermodynamic modelling of bentonite-groundwater interaction and implications for near field chemistry in a repository for spent fuel. SKB TR 92-37.	
DYLAN and Nag equation solvers and PHREEQC	Temperature effects on solubility and migration of calcium sulphates, calcite, silicon in the buffer.	Arcos, D., Bruno, J., Benbow, S., and Takase, H., 1999. Behaviour of bentonite accessory minerals during the thermal stage. SKB TR-00-06.	
Analytical	Thermodynamic model of the effects of salinity on swelling pressure.	Karnland, O., 1997. Bentonite swelling pressure in strong NaCl solutions. Correlation between model calculation and experimentally determined data. SKB TR 97-31.	

SR 97 safety assessment			SR-Can safety assessment
Code	**Function**	**References in SKB (1999a and b)**	**Additional/alternative codes/analysis referred to in SKB (2003; 2004)**
?	Buffer illitization.	Hökmark H., 1996. Canister positioning. Stage 1: Thermomechanical nearfield rock analysis. SKB AR D-96-014.	
		Canister defect scenario	
Radiation-related			
Scale 4.4	Canister criticality analysis.	Agrenius, L., 1999. SKB R-99-52. (in Swedish)	Scale 4.4 criticality calculations: Agrenius, 2002. Criticality safety calculations of storage canisters. SKB TR-02-17.
?	Canister criticality analysis.	Efraimsson, H., 1996. SKB PPM 95-3430-04. (in Swedish) Efraimsson, H., 1996. SKB PPM 96-3430-06. (in Swedish)	
Hydromechanical			
Unnamed canister corrosion code - ABAQUS 5.5 for stress	Hydromechanical evolution in a canister, including mechanical effects of corrosion products.	Bond A.E., Hoch, A.R., Jones, G.D., Tomczyk, A., Wiggin, R.M., and Worraker, W.J., 1997. Assessment of a spent fuel disposal canister. Assessment studies for a copper canister with cast steel inner component. SKB TR-97-19.	
Unnamed codes	Hydromechanical evolution in a canister.	Takase, H., Benbow, S., and Grindrod, P., 1999. Mechanical failure of SKB spent fuel disposal canisters - mathematical modelling and scoping calculations. SKB TR-99-34.	
Analytical (but GAMMON proposed)	Gas migration through the buffer from a canister.	Wikramaratna, R.S., Goodfield, M., Rodwell, W.R., Nash, P.J., and Agg, P.J., 1993 A preliminary assessment of gas migration from the Copper/Steel Canister. SKB TR-93-31.	
Chemical			
?	Fuel dissolution rate - radiolytic oxidation.	Eriksen, T., 1999. Radiolysis of water within a ruptured fuel element. SKB TR-99-XX (in preparation). Eriksen, T., 1996. Radiolysis of water within a ruptured fuel element. SKB PR U-96-29.	

SR 97 safety assessment			SR-Can safety assessment
Code	**Function**	**References in SKB (1999a and b)**	**Additional/alternative codes/analysis referred to in SKB (2003; 2004)**
Macksima-Chemist	Radiolysis model.	Carver, M.B., Hanley, D.V., and Chaplin, K.R., 1979. "Macksima-Chemist". A program for mass action kinetics simulation by automatic chemical equation manipulation and integration using stiff techniques, AECL 6413.	
EQ3NR	Solubility calculations – equilibrium model.	Bruno, J., Cera, E., de Pablo, J., Duro, L., Jordana, S., and Savage, D., 1997. Determination of radionuclide solubility limits to be used in SR 97. Uncertainties associated to calculated solubilities. SKB TR-97-33.	
Hydraulic			
HYDRASTAR	3D finite difference model for stochastic continuum simulation of groundwater flow - primary local-scale model.	Norman, S., 1991. Verification of HYDRASTAR - A code for stochastic continuum simulation of groundwater flow. SKB TR-91-27. Morris, S.T. and Cliffe, K.A., 1994. Verification of HYDRASTAR: Analysis of hydraulic conductivity fields and dispersion. SKB TR-94-21. Walker, D. (ed), Eriksson, L., and Lovius, L., 1996. Analysis of the Äspö LPT2 pumping test via simulation and inverse modelling with HYDRASTAR. SKB TR-96-23. Walker, D. and Gylling, B., 1998. Site-scale groundwater flow modelling of Aberg. SKB TR-98-23. Gylling, B., Walker, D., and Hartley, L., 1999. Site-scale groundwater flow modelling of Beberg. SKB TR-99-18. Walker, D. and Gylling, B., 1999. Site-scale groundwater flow modelling of Ceberg. SKB TR-99-13 Widén, H. and Walker, D., 1999. SR 97 Alternative Modelling Project: Stochastic continuum modelling of Aberg. SKB R-99-42 Norman, S., 1992. HYDRASTAR – a code for stochastic simulation of groundwater flow. SKB TR 92-12.	SKB plans to replace HYDRASTAR with CONNECTFLOW and DarcyTools: Jaquet, O. and Siegel, P., 2004. Local scale modelling of density-driven flow for the phases of repository operation and post-closure at Beberg, SKB R-04-46. Hartley, L., Cox, I., Holton, D., Hunter, F., Joyce, S., Gylling, B., Lindgren, M., 2004. Groundwater flow and radionuclide transport modelling using CONNECTFLOW in support of the SR-Can assessment. SKB R-04-61. Marsic, N., Hartley, L., Jackson, P., Poole, M., and Morvik, A., 2001. Development of hydrogeological modelling tools based on NAMMU, SKB R-01-49. Marsic, N., Hartley, L., Sanchez-Friera, P., and Morvik, A., 2002. Embedded regional /local scale model of natural transients in saline groundwater flow. Illustrated using the Beberg site, SKB R-02-22.

SR 97 safety assessment			**SR-Can safety assessment**
Code	**Function**	**References in SKB (1999a and b)**	**Additional/alternative codes/analysis referred to in SKB (2003; 2004)**
			Svensson, U., 2002. DarcyTools – Software description and documentation, version 1.0, SKB TS-02-05. Svensson, U., 2002. DarcyTools – Concepts, methods, equations and tests, version 1.0, SKB TS-02-06. Other hydrological analysis: Holmén J, Stigsson M, Marsic N, Gylling B, 2003. Modelling of groundwater flow and flow paths for a large regional domain in northeast Uppland. SKB R-03-24. Holmén J, Forsman J, 2004. Flow of groundwater from great depths in the near surface deposits; modelling of a local domain in northeast Uppland. SKB R-04-31. DHI, 2003. DHI Water and Environment. MIKE SHE User Manual - Water Movement.
CHAN3D	Channel network model for simulation of groundwater flow and transport.	Gylling, B., Moreno, L., and Neretnicks, I., 1999. SR 97 Alternative Models Project: Performance assessment using CHAN3D. SKB R-99-44.	Moreno, L., Crawford, J., and Neretnieks, I., 2003. Modelling of solute transport under flow conditions varying in time using CHAN3D, MRS 2003. Moreno, L., Crawford, J., and Neretnieks, I., 2003. Modelling of solute transport under varying flow conditions. In Proceedings of Scientific Basis for Nuclear Waste Management, Kalmar, Sweden.

SR 97 safety assessment			SR-Can safety assessment
Code	**Function**	**References in SKB (1999a and b)**	**Additional/alternative codes/analysis referred to in SKB (2003; 2004)**
Fracman/MAFIC/PAWorks	Software package for stochastic simulation of groundwater flow and transport in discrete fracture networks.	Dershowitz, B., Follin, S., Andersson, J., and Eiben, T., 1999. SR 97 Alternative Models Project: Discrete fracture network modeling for performance assessment of Aberg. SKB R-99-43	
NAMMU	Finite element continuum model - flow and transport at Beberg.	Marsic, N., Gylling, B., Grundfelt, B., and Hartley, L., 2000. Modelling of the site scale hydrogeological situation at Beberg using NAMMU. SKB R-00-14.	
NAMMU	Regional model for Beberg.	Hartley, L., Boghammar, A., and Grundfelt, B., 1998. Investigation of the large scale regional hydrogeological situation at Beberg. SKB TR-98-24.	
?	Local-scale transient model for Aberg.	Svensson, U., 1999. A numerical simulation of the origin and composition of the groundwater below Äspö. SKB R-99-39.	
NUCTRAN	Transport in the backfill.	Moreno, L., 2000. Impact of the water flow rate in the tunnel on the release of radionuclides. SKB TR-00-03.	
Analytical (but GAMMON proposed)	Gas migration through the geosphere.	Wikramaratna, R.S., Goodfield, M., Rodwell, W.R., Nash, P.J., and Agg, P.J., 1993 A preliminary assessment of gas migration from the Copper/Steel Canister. SKB TR-93-31.	
Biosphere			
ACTIVI	Transport model for turnover of radionuclides in the ecosystem and model of exposure to radiation - both in program ACTIVI (a BIOPATH subroutine).	Bergström, U., Nordlinder, S., and Aggeryd, I., 1999. Models for dose assessments for various biosphere types. SKB TR-99-14. Bergström, U., Edlund, O., Evans, S., and Röjder, B., 1982. BIOPATH - A computer code for calculation of the turnover of nuclides in the biosphere and the resulting doses to man. STUDSVIK/NW-82/261.	CoupModel: Jansson P-E, Karlberg L, 2004. Coupled heat and mass transfer model for soil-plant atmosphere systems. Royal Institute of Technology, Dept of Civil and Environmental Engineering., Stockholm, Sweden, 435 pp. Lindborg R, Kautsky U, 2004. in manus. Ecosystem modelling in the Forsmark area – results from two workshops modelling Eckarfjärden and Bolundsfjärden catchment areas. SKB R-04-xx.

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PRISM	Variation in eco-system specific dose conversion factors (EDF).	Gardner, R.H., Röjder, B., and Bergström, I., 1983. PRISM - A systematic method for determining the effect of parameter uncertainties on model predictions. STUDSVIK/NW-83/555.	
Radionuclide transport			
COMP23	Near-field model - compartment model based on NUCTRAN - release of radionuclides from fuel and transfer to the rock.	Romero, L., 1995. The near-field transport in a repository for high-level nuclear waste, PhD Thesis, TRITA-KET R21, The Royal Institute of Technology, Stockholm, Sweden. Romero, L., Thompson, A., Moreno, L., Neretnicks, I., Widén, H., Boghammar, A., and Thompson, A., 1999. COMP23, Nuctran user's guide. PROPER Version 1. 1.6. SKB R-99-64. Moreno, L. and Gylling, B., 1998. Equivalent flow rate concept in near field transport model COMP23. SKB R-98-53. Lindgren, M. and Widén, H., 1998. Discretization in COMP23 for SR 97 SKB R-98-03. Andersson, J., Hermansson, J., Elert, M., Gylling, B., Moreno, L., and Selroos, J-O., 1998. Derivation and treatment of the flow wetted surface and other geosphere parameters in the transport models FARF31 and COMP32 for use in safety assessment. SKB R-98-60.	Cliffe, K.A., 2004. COMP23 v1.2.1 Users manual. SKB R-04-64.
FARF31	Far-field model - transport of radionuclides through the rock - 1D stream tubes – double-porosity model.	Norman, S. and Kjellbert, N., 1990. FARF31 - A far field radionuclide migration code for use with the PROPER package. SKB TR-90-01. Andersson, J., Hermansson, J., Elert, M., Gylling, B., Moreno, L., and Selroos, J-O., 1998. Derivation and treatment of the flow wetted surface and other geosphere parameters in the transport models FARF31 and COMP32 for use in safety assessment. SKB R-98-60.	FVFARF colloid transport model: Vahlund F, Hermansson H, 2004. FVFARF - a direct numerical approach to solving the transport equations for radionuclide transport in fractured rock. SKB R-04-xx. Elert, M., Gylling, B., and Lindgren, M., 2004. Assessment model validity document FARF31. SKB Report R-04-51.

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BIO42	Dose model - turnover of radionuclides in the biosphere.	BIOMOVS, 1993. Final report. BIOMOVS Technical report 15, SSI BIOMOVS 11, 1996. An overview of the BIOMOVS 11 study and its findings, TRI7 Swedish Radiation Protection Institute (SSI) VAMP 1996. Validation of models using Chernobyl fallout data from southern Finland. Scenario S. Second report of the VAMP Multiple Pathways Assessment Working Group. IAEA-TECDOC-904, International Atomic Energy Agency (IAEA), Vienna.	Jones J, Vahlund F, Kautsky U, 2004. Tensit – A novel probabilistic simulation tool for safety assessments – Tests and verifications using biosphere models. SKB TR-04-07.
PROPER, COMP23, FARF31, BIO42	Details of transport calculations.	Lindgren, M. and Lindström, F., 1999. SR 97 - Radionuclide transport calculations. SKB TR-99-23.	
?	Analytical model for release and transport of radionuclides in canister and buffer.	Hedin, A., 1999. An analytic model for radionuclide releases in the near-field, SKB Internal PM 1999.	Hedin, A., 2002. Integrated Analytic Radionuclide Transport Model for a Spent Nuclear Fuel Repository in Saturated Fractured Rock. Nuclear Technology 138 2 179 (2002). Hedin, 2003. Probabilistic dose calculations and sensitivity analyses using analytic models. Reliability Engineering and System Safety 79 (2003) 195–204.
?	Radionuclide transport with gas and particles.	Neretnieks, I. and Ernstson, M-L., 1997. A note on radionuclide transport by gas bubbles, Mat. Res. Soc. Symp. Proc., vol. 465, pp. 855-862.	

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		Climate scenario	
General			
ACLIN	Astronomical Climate Index - calculates global climate index.	Kukla, G., Berger, A., Lotti, R., and Brown, J.P., 1981. Orbital signatures of interglacials. Nature, 290(5804), 295-300.	BIOCLIM, 2001. Global climatic features over the next million years and recommendation for specific situations to be considered. BIOCLIM Deliverable 3, EC-CONTRACT : FIKW-CT-2000-00024 BIOCLIM, 2003. Continuous climate evolution scenarios over western Europe (1,000 km scale). BIOCLIM Deliverable D7, EC-CONTRACT: FIKW-CT-2000-00024. Fastook J L, Chapman J E, 1989. A map plane finite-element model: Three modelling experiments. Journal of Glaciology 35 (119), 48–52. Fastook J L, 1994. Modelling the Ice Age: The Finite-Element Method in Glaciology. Computational Science and Engineering 1 (1), 55–67. Fastook, J L, Holmlund, P, 1994. A glaciological model of the Younger Dryas event in Scandinavia. Journal of Glaciology 40 (134), 125–131.
Imbrie & Imbrie model	Calculates global ice volume (ice sheet dynamics).	Imbrie, J. and Imbrie, J.Z., 1980. Modelling the Climatic Response to Orbital Variations. Science, Vol 207, 943-953.	

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LLN	Louvaine-la-Neuve 2D northern hemisphere climate model – ice-sheet model.	Gallée, H., van Ypersele, J.P., Fichefet, Th., Tricot, Ch., and Berger, A., 1991. Simulation of the Last Glacial Cycle by a Coupled, Sectorially Averaged Climate-Ice Sheet Model. 1. The Climate Model. journal of Geophysical Research, vol. 96, NO D7, 13,139-13,161. Gallée, H., van Ypersele, J.P., Fichefet, Th., Tricot, Ch., and Berger, A., 1992. Simulation of the Last Glacial Cycle by a Coupled, Sectorially Averaged Climate-Ice Sheet Model. 2. Response to Insolation and $C0_2$ Variations. Journal of Geophysical Research, vol 97, NO D14, 15,713-15,740 Berger, A. and Loutre, M.F., 1997. Palaeoclimate Sensitivity to $C0_2$ and insolation Ambio Vol 26, No 1, 32-37.	
Imbrie & Imbrie, LLN, and ACLIN	Climate change modelling.	Morén, L. and Påsse, T., 1999. Climate and shoreline in Sweden during Weichsel and the next 150,000 years. SKB TR-01-19.	
Analytical	Shore-line displacement model based on arctan functions.	Påsse, T., 1996. A mathematical model of the shore level displacement in Fennsoscandia. SKB TR 96-24. Påsse, T., 1997. A mathematical model of past, present and future shore level displacement in Fennsoscandia. SKB TR 97-28.	
Unnamed code	Scandinavian ice-sheet model.	Boulton, G.S. and Payne, A., 1992. Simulation of the European ice sheet through the last glacial cycle and prediction of future glaciations. SKB TR 93-14. Boulton, G.S., Hulton, N., and Vautravers, M., 1995. Ice-sheet models as tools for palaeoclimatic analysis: the example of the European ice sheet through the last glacial cycle. Annals of Glaciology 21, 103-110. Boulton, G.S., Kautsky, U., Morén, L., and Wallroth, T., 2001. Impact of long-term climate change on a deep geological repository for spent nuclear fuel SKB TR-99-05.	Näslund, J.O. and Jansson, P., 2003. Project plan: Basal conditions and hydrology of continental ice sheets, Svensk Kärnbränslehantering AB. Näslund, J.O., Rodhe, L., Fastook, J., and Holmlund, P., 2003. New ways of studying ice sheet flow directions and glacial erosion by ice sheet modelling – examples from Fennoscandia. Quaternary, Science Reviews 22(2–4):89–102.

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		Mangerud, J., 1991. The Scandinavian ice sheet through the last interglacial/glacial cycle. In Frenzel B ed Klimatgeschichtliche Probleme der letzen 130,000 Jahre. Stuttgart, Fisher Verlag, 307-330. Fredén, C. (ed), 1994. National Atlas of Sweden – Geology. Almqvist & Wiksell International, Stockholm. ISBN 91-87760-28-2.	Hartikainen J, Mikkola M, 2003. Thermomechanical modelling for freezing of solute saturated soil. To appear in Proceedings of the IUTAM-Symposium on the mechanics of physicochemical and electromechanical interactions in porous media. Hartikainen J, 2004. Estimation of Permafrost Depth at Forsmark. Helsinki University of Technology Research Reports of the Laboratory of Structural Mechanics, TKK-RM-04-05.
Hydraulic			
Analytical	Groundwater flow beneath ice sheets.	Boulton, G.S., Zatsepin, S., and Maillot, B., 2001. Analysis of groundwater flow beneath ice sheets. SKB TR-01-06.	CONNECTFLOW: Jaquet, O. and Siegel, P., 2003. Groundwater flow and transport modelling during a glaciation period. SKB R-03-04.
?	Geosphere (flow) evolution at Aberg.	Svensson, U., 1999. Subglacial groundwater flow at Äspö as governed by basal melting and ice tunnels. SKB R-99-38. Svensson, U., 1999. A numerical simulation of the origin and composition of the groundwater below Äspö. SKB R-99-39.	
Mechanical			
?	Glacial loading.	Stephansson, O., 1993. Rock stress in the Fennoscandian Shield. In. Hudson J A (ed) Comprehensive Rock Engineering, Vol 3, Rock Testing and Site Characterisation, pp 445-459, Pergamon Press.	3DEC may be used for general analysis of load cases. Global isostatic adjustment (GIA) modelling planned.
UDEC	Near-field effects of glaciers.	Rosengren, L. and Stephansson, O., 1990. Distinct element modelling of the rock mass response to glaciation at Finnsjön, central Sweden. SKB TR 90-40.	

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3DEC	Far-field effects of glaciers.	Hansson, H., Stephansson, O., and Shen, B., 1995. SITE-94. Far-field rock mechanics modelling for nuclear waste disposal. SKI Report 95:40.	
3DEC	Shear movements during glaciation.	Shen, B. and Stephansson, O., 1990. 3DEC mechanical and thermomechanical analysis of glaciation and thermal loading of a waste repository. SKI Report 90:3.	
Chemical			
PHREEQC and ARASE	Geochemical effects of ice-sheet melting.	Guimera, J., Duro, L., Jordana, S., and Bruno, J., 1999. Effects of ice melting and redox front migration in fractured rocks of low permeability. SKB TR-99-19.	
M3	Mixing calculations at an ice front.	Laaksoharju, M., Gurban, I., and Andersson, C., 1998. Summary of hydrochemical conditions at Aberg, Beberg and Ceberg. Intera KB, Sollentuna, Sweden. SKB TR-98-03. Laaksoharju, M., Gurban, I., and Andersson, C., 1999. Indications of the origin and evolution of the groundwater at Palmottu. The EU Palmottu natural analogue project. SKB TR-99-03 (not published).	Laaksoharju, M., Skårman, C., and Skårman, E., 1999. Multivariate mixing and mass balance (M3) calculations, a new tool for decoding hydrogeochemical information, Appl. Geochem. 14 (1999) 861–871. Rock-water interaction modelling using PHREEQC.
Radionuclide transport			
PHOENICS	Groundwater flow and radionuclide transport at Aberg.	Svensson, U., 1997. A regional analysis of groundwater flow and salinity distribution in the Äspö area. SKB TR 97-09.	
?	Groundwater flow and radionuclide transport at Aberg.	Svensson, U., 1999. Subglacial groundwater flow at Äspö as governed by basal melting and ice tunnels. SKB R-99-38. Svensson, U., 1999. A numerical simulation of the origin and composition of the groundwater below Äspö. SKB R-99-39.	

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Tectonics – earthquake scenario			
Mechanical			
Analytical	Strains due to glacial loading/unloading.	Muir Wood, R., 1993. A review of the seismotectonics of Sweden. SKB TR 93-13. Wallroth, T., 1997. SKB R-97-11. (in Swedish)	
POLY3D	Canister damage due to earthquakes (Aberg, Beberg, Ceberg). Fracture displacements. Fracman used to generate the discrete fracture network.	LaPointe P., Cladouhos T., and Follin, S., 1999. Calculation of displacements on fractures intersecting canisters induced by earthquakes. Aberg, Beberg and Ceberg examples. SKB TR-99-03. LaPointe, P., Wallman, P., Thomas, A., and Follin, S., 1997. A methodology to estimate earthquake effects on fractures intersecting canister holes. SKB TR 97-07. Munier, R., Sandstedt, H., and Niland, L., 1997. SKB R-97-09. (in Swedish)	Further application of POLY3D to evaluate fracture displacements: LaPointe, P., Cladouhos, T., Outters, N., and Follin, S., 2000. Evaluation of the conservativeness of the methodology for estimating earthquake-induced movement of fractures intersecting canisters. SKB TR-00-08. Application of ABAQUS to evaluate fracture displacements: Börgesson, L., Johannesson, L.-E., and Hernelind, J., 2004. Earthquake induced rock shear through a deposition hole. Effect on the canister and the buffer, SKB TR-04-02. Other: Munier R, Hökmark H, 2004. Respect distances. Rationale and means of computation. R-04-17. Hökmark H, Christiansson M, Baker C. In prep. Numerical handling of earthquakes in the vicinity of the repository.

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?	Plastic strain on copper canister.	Börgesson, L., 1992. Interaction between rock, bentonite buffer and canister. FEM calculations of some mechanical effects on the canister in different disposal concepts. SKB TR 92-30.	
		Human Actions Scenarios	
?	Dose from drilling into canister.	Bergström, U., Edlund, O., Nordlinder, S., 1995. Human activities affecting the integrity of a deep geological repository for nuclear waste – Radiological risks from intrusion. SKB PR U-96-06.	

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